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ADMET Predictor(TM) Output file  4/7/2022  5:42:22 PM

Input File Name =
S:\AGO\PD_SolidDose\FormDev_NewProducts\Projects\Steptoe\Conformer3D_CID_9444
(1).sdf

Default Hayduk-Laudie diffusivity [cm^2/s x 10^5] model
Default S+MDCK permeability [cm/s x 10^7] model
Default S+Peff permeability [cm/s x 10^4] model
Default Meylan solubility [mg/mL] model
Default S+Sw solubility [mg/mL] model
Default S+BBB permeability model
Default S+PrUnbnd percent unbound model
Default S+Vd volume of distribution [L/kg] model
ADMET Risk rules from c:\program files\simulations plus,
inc\admet_predictor\Default.ro5
pH for ionization descriptors = 7.4
pH for pH-sensitive models = 7.4

*molname        PUBCHEM_COMPOUND_CID    PUBCHEM_CONFORMER_RMSD
PUBCHEM_CONFORMER_DIVERSEORDER  PUBCHEM_MMFF94_PARTIAL_CHARGES
PUBCHEM_EFFECTIVE_ROTOR_COUNT   PUBCHEM_PHARMACOPHORE_FEATURES
PUBCHEM_HEAVY_ATOM_COUNT        PUBCHEM_ATOM_DEF_STEREO_COUNT
PUBCHEM_ATOM_UDEF_STEREO_COUNT  PUBCHEM_BOND_DEF_STEREO_COUNT
PUBCHEM_BOND_UDEF_STEREO_COUNT  PUBCHEM_ISOTOPIC_ATOM_COUNT
PUBCHEM_COMPONENT_COUNT PUBCHEM_CACTVS_TAUTO_COUNT      PUBCHEM_CONFORMER_ID
PUBCHEM_MMFF94_ENERGY   PUBCHEM_FEATURE_SELFOVERLAP     PUBCHEM_SHAPE_FINGERPRINT
PUBCHEM_SHAPE_MULTIPOLES        PUBCHEM_SHAPE_SELFOVERLAP
PUBCHEM_SHAPE_VOLUME    PUBCHEM_COORDINATE_TYPE MeltingPoint    Orig.Order
Acid_Pred_pKa   Base_Pred_pKa   DiffCoef        MlogP   S+logP  Outsider_of_S+logP
S+logD  S+Peff  Outsider_of_S+Peff      S+Pavg  Outsider_of_S+Pavg      S+MDCK
Outsider_of_S+MDCK      S+Sw    Outsider_of_S+Sw        S+pH    S+IS    S+SF
S+Sp    S+BBB   Outsider_of_S+BBB       S+PrUnbnd       Outsider_of_S+PrUnbnd
S+Vd    Outsider_of_S+Vd        TOX_MRTD        Outsider_of_TOX_MRTD
TOX_ER_Filter   Outsider_of_TOX_ER_Filter       TOX_ER  Outsider_of_TOX_ER
TOX_FHM Outsider_of_TOX_FHM     TOX_hERG        Outsider_of_TOX_hERG    TOX_BRM_Rat
Outsider_of_TOX_BRM_Rat TOX_BRM_Mouse   Outsider_of_TOX_BRM_Mouse       S+HIVI-ST
Outsider_of_S+HIVI-ST   S+HIVI-TC       Outsider_of_S+HIVI-TC   SimHIA_1
SimHIA_10       SimHIA_100      SimHIA_1000     ADMET_Risk      ADMET_Code
Formula MWt     MolVol  VMcGowan        N_Atoms N_Carbon        N_Ntrgen
N_Oxygen        N_Phsphr        N_Sulfur        N_Fluorn        N_Chlorn
N_Bromin        N_Iodine        N_Halogen       N_Nonorgn       N_Metal N_Bonds
N_FrRotB        F_SgleB F_DbleB F_TpleB F_AromB F_AFRBWF        N_Rings N_AromR
N_AlipR N_Pisyms        N_Kekule        X0      X1      X2      Kappa1  Kappa2
Kappa3  Wiener  SsCH3   SssCH2  SsssCH  SsssssC SdCH2   SdsCH   SdssC   SaaCH
SaasC   SaadC   SaaaC   StCH    SddC    StsC    SsssssN SdsssN  SsNH2   SssNH
SsssN   SdNH    SdsN    SdssN   SaaN    SaaNH   SaasN   SddsN   SaadN   SaaaN   StN
StsN    StdN    SsOH    SssO    SsO-    SdO     SaaO    SdsssP  SdssPH  SsPH2
SssPH   SsssP   SsssssP SddssS  SsSH    SssS    SsssssssS       SdssS   SsssS   SdS
SaaS    SsF     SsCl    SsBr    SsI     SHsOH   SHdNH   SHsNH2  SHssNH  SHsSH
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SHCH_321        SHdCH2  SHdsCH  SHaaCH  SHtCH   S_unknown       AlHdrxl_-OH
ArHdrxl_-OH     Carbonyl_C=O    Ether___-O-     PriAmine_-NH2   PriAmAli_-NH2
PriAmAro_-NH2   SecAmine_>NH    TerAmine_>N-    QuaAmine_>[N+]< ArNitrog_=N-
Imine___=N-     Nitrile_C#N     Isocynd_[N+]#[C-]       Thiol___-SH
ThioCrbl_C=S    Sulfide_-S-     Slfonium_>[S+]- Phsphine_>P-    HydxlAmn_>N-O-
Oxime___=N-O-   Nitroso_-N=O    Hdrzine_>N-N<   Hdrzone_=N-N<   Azo_____-N=N-
Diazo___-[N+]#N ThioAmin_>N-S-  Disulfde_-S-S-  Sulfoxde_>S=O   Thioxime_=N-S-
Nitro___-NO2    Nitrite_-O-N=O  Ntrosam_>N-N=O  Azoxy___-N(=O)=N-
Azide___-N=N#N  Sulfone_>S(=O)=O        Sulfinat_S(=O)O-        Phsporat_P(=O)O-
Triazo__-N-N-N- Oxadiazo_-N-O-N-        Thiadiaz_-N-S-N-        Triazene_-N=N-N-
Nitrate_-O-NO2  NNitro__>N-NO2  Sulfonat_-SO3-  Sulfite_-SO3<   Sulfonmd_-SO2-N<
PriSlfmd_-SO2-NH2       Phsponat_-PO3<  SPhspnat_-SPO2< Phspite_-OPO2<
Tetrazo_-NNNN-  Oxdzoxde_-N(=O)ON-      NOHydxam_-N(N=O)OH      Sulfamid_>NSO2N<
Sulfate_-OSO3   ThioSulf_-SSO3  Phspate_O=PO3<- PhspatS_O=PS(k)O(3-k)<-
SPhspat_S=PO3<- SPhspatS_S=PS(k)O(3-k)<-        PhspatN_O=PN(n)O(3-n)<<<
SPhspatN_S=PN(n)O(3-n)<<<       PhsptSN_O=PS(k)N(n)O(3-n-k)<<
SPhsptSN_S=PS(k)N(n)O(3-n-k)<<  Diphspat_O=PO2-O-PO2=O
Triphspt_O=PO2-O-PO(=O)-OPO2=O  AlCbxyl_-COOH   ArCbxyl_-COOH   Ester___C(=O)OC
Amide___C(=O)N< Thioamd_C(=S)N< Amidine_C(=N-)N<        Isocyant_-N=C=O
Thiocynt_-S-C#N Isothcnt_-N=C=S Urea____>NC(=O)N<       Carbmte_>NC(=O)O<
Guandne_>NC(=N-)N<      Imide___O=C(N-)C=O      Barbitur_C1C(=O)NC(=O)NC1=O
Unknown_        M_CX    M_NO    M_PRX   M_UB    M_HB    M_POL   M_AMP   M_ALK
M_RNG   M_QN    M_NO2   M_NCS   M_BLM   AlphaAA PrAlphAA        AlphaAE PrAlphAE
Steroid H_AlAlco        H_AlAcid        H_AlAmin        H_ArAcid        H_Phenol
H_AlPyri        H_Azo   H_Nitrle        H_HCarb H_Nitro H_SO2   H_FAlkan
H_PAH   H_MultiN        H_AmAcid        RgGrav__3D      RgGeom__3D      RadMax__3D
Propr1__3D      MIRxx___3D      MIRyy___3D      MIRzz___3D      SM2xx___3D
SM2yy___3D      SM2zz___3D      BoxX____3D      BoxY____3D      BoxZ____3D
DStokes_3D      Propr2__3D      Grav3___3D      TotASA__3D      PolASA__3D
NpoASA__3D      SolvE___3D      SolvEMt_3D      PEoED___3D      PEoEDIa_3D
PEoEDIb_3D      PEoEDIIa3D      PEoEDIIb3D      T_Rgrav T_Rgeom T_Radmax
T_Dipole        T_Grav3 FormalQ IHB     PHB     HBD     HBA     HBDo    HBAo
HBDn    HBAn    HBDch   HBAch   HBDoch  HBAoch  HBDnch  HBAnch  HBAsa___3D
HBAwsa__3D      PosASA__3D      NegASA__3D      Dipole__3D      ABSQ    ABSQon
MaxQ    MinQ    NPA_ABSQ        NPA_AQon        NPA_MaxQ        NPA_MinQ
NPA_Q1  NPA_Q2  NPA_Q3  NPA_Q4  NPA_Q5  NPA_Q6  EqualChi        N_Electr
PolarizG        PolarizM        N_IoAcAt        N_IoBaAt        AcidAtoms
BaseAtoms       FAnion  FCation FUnion  FZwitter        QAvgNeg QAvgPos F_NLP
F_HBP
9444    9444    0.6     1 12 13 7 5 14 10 2 6 11 4 9 8 3        23 1 -0.56 10 0.28
11 0.28 12 0.28 13 0.58 14 0.28 15 0.84 16 0.45 17 0.71 2 -0.68 24 0.4 25 0.4 26
0.06 27 0.4 28 0.4 29 0.4 3 -0.68 4 -0.68 5 -0.57 6 -0.42 7 -0.66 8 -0.66 9 -0.85
3       12 1 1 acceptor 1 2 acceptor 1 2 donor 1 3 acceptor 1 3 donor 1 4 acceptor
1 4 donor 1 5 acceptor 1 7 donor 1 9 donor 5 1 10 11 12 13 rings 6 6 7 8 15 16 17
rings   17      4       0       0       0       0       1       3       1.#INF
50.9521 60.962  10608611 8 18411694409049253760 11132069 177 18412541020444494778
12138202 97 18115012001220561597 12500047 106 18337105674893126407 12932764 1
17967523554309708816 12969540 114 17969481746681867365 13024252 1
16008756779798805865 14115302 16 183371210766   300.58 6.14 2.47 0.84 3.95 0.5 0.04
1.55 0.49 -1.36 0.1 -0.24 -0.17 0.57    635.496 168.2   2 5 10  0.0     1
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 3.14;-1.95;-3.60;-7.33 1.01    -1.1    -2.09   0       -2.09   0.14    0
0.51    0       59.56   0       1.44E+01        0       7.96    1.44E+01
1.21E+01        1.44E+01        Low     1       75.39   0       0.67    0
More_than_3.16  0       Nontoxic        0       0.0001  1       2429.43 1
3.51    1       22.57   0       957.72  1       3.8     0       4.11    0
                        3.0     LP_Pr_Hd_       C8H12N4O5       244.21  189.
243.5   17      8       4       5       0       0       0       0       0       0
0       0       0       18      2       0.61    0.06    0.00    0.33    0.29    2
1       1       5       1       12.58   8.04    7.35    13.43   5.33    2.56    496
0.0     -0.4729 -4.735  0.0     0.0     0.0     0.0     1.0605  -0.1963 -0.7571 0.0
0.0     0.0     0.0     0.0     0.0     5.2133  0.0     0.0     0.0     0.0     0.0
6.9566  0.0     0.9027  0.0     0.0     0.0     0.0     0.0     0.0     28.0899
5.134   0.0     11.4709 0.0     0.0     0.0     0.0     0.0     0.0     0.0     0.0
0.0     0.0     0.0     0.0     0.0     0.0     0.0     0.0     0.0     0.0     0.0
7.9055  0.0     1.7543  0.0     0.0     5.978   0.0     0.0     1.6434  0.0     0
3       0       0       1       1       0       1       0       0       0       1
0       0       0       0       0       0       0       0       0       0       0
0       0       0       0       0       0       0       0       0       0       0
0       0       0       0       0       0       0       0       0       0       0
0       0       0       0       0       0       0       0       0       0       0
0       0       0       0       0       0       0       0       0       0       0
0       0       0       0       0       0       0       0       0       0       1
0       0       0       0       0       8.00    9       8       4       0       2
0.00    0       1       0.00    0       0.00    0       0       0       0       0
0       0       0       0       0       0       0       0       0       0       0
0       0       0       0       0       2.89E+00        2.84E+00        4.75E+00
3.37E+00        4.81E-01        3.64E-01        1.54E-01        3.73E-02
2.71E-01        6.92E-01        2.11E+00        5.42E+00        7.96E+00
6.92E-01        3.60E-01        1.34E+01        3.79E+02        2.07E+02
1.72E+02        -2.20E+01       1.84E+01        16      6       2       10      4
2.89E+00        2.82E+00        4.80E+00        1.73E+00        1.50E+01        0
0       0       4       8       3       5       1       3       2.2     -4.95
1.41    -3.09   0.8     -1.87   2.07E+02        -1.36E+02       1.72E+02
2.07E+02        1.86E+00        0.47    0.47    0.24    -0.08   10.96   5.42    0.8
-0.8    -2.75   2.5     -1.67   0.85    -0.38   0.06    5.63    128     21.97
21.33   0       4       None    9(-NH2)6(-Naa)7(aNa)8(aNa)      0.0     0.0001
0.9999  0.0     0.0     0.0001  0.7647  0.2941
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