Dyphylline

Other names:

(1,2-Dihydroxy-3-propyl)thiophyllin
(rac)-Diprophylline
1,3-Dimethyl-7-(2,3-dihydroxypropyl)xanthine
1H-Purine-2,6-dione, 7-(2,3-dihydroxypropyl)-3,7-dihydro-1,3-dimethyl-
7-(2,3-Dihydroxypropyl)-1,3-dimethylxanthine
7-(2,3-Dihydroxypropyl)-3,7-dihydro-1,3-dimethyl-1H-purine-2,6-dione
7-(2,3-Dihydroxypropyl)-3,7-dihydro-1,3-dimethyl-1H-purine-2,6-dione (dyphylline)
7-(2,3-Dihydroxypropyl)theophylline
7-(2,3-Dioxypropyl)theophylline
7-(2,3-dihydroxypropyl)-1,3-dimethyl-3,7-dihydro-1H-purine-2,6-dione
7-(«beta»,«gamma»-Dihydroxypropyl)theophylline
7-(Â«betaÂ»,Â«gammaÂ»-Dihydroxypropyl)theophylline
AFI-Phyllin
Aristophyllin
Asthmolysin
Astmamasit
Astrophyllin
Circain
Circair
Cor-Theophylline
Coronal
Coronarin
Corphyllin
Dihydroxypropyl theophylline
Dihydroxypropyl theopylin
Dilor
Diphyllin
Diphylline
Diprofillin
Diprofilline
Diprophyllin
Diprophylline
Dipropylline
Droxine
Dyflex
Glyfyllin
Glyphyllin
Glyphylline
Hidroxiteofillina
Hiphyllin

Hyphylline
Iphyllin
Isophyllen
Liactemin
Lufyllin
Neo-Vasophylline
Neophyl
Neophyllin
Neophylline
Neostenovasan
Neothyllin
Neothylline
Neotilina
Neufil
Neutrafil
Neutrafillina
Neutraphyllin
Neutraphylline
Neutroxantina
Propyphyllin
Protheophylline
Purifilin
Silbephyllin
Silbephylline
Solufilin
Solufyllin
Soluphyllin
Synthophylline
Tefilan
Teofen
Theal
Theal ampules
Thefylan
Theophylline, 7-(2,3-dihydroxypropyl)-

Inchi: InChI=1S/C10H14N4O4/c1-12-8-7(9(17)13(2)10(12)18)14(5-11-8)3-6(16)4-15/h5-6,15-16

InchiKey: KSCFJBIXMNOVSH-UHFFFAOYSA-N

Formula: C10H14N4O4

SMILES: Cn1c(=O)c2c(ncn2CC(O)CO)n(C)c1=O

Mol. weight [g/mol]: 254.24

CAS: 479-18-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.17		Aqueous Solubility Prediction Method
log10ws	-0.17		Estimated Solubility Method
log10ws	0.12		Aqueous and cosolvent solubility data for drug-like organic compounds
logp	-2.213		Crippen Method
mcvol	176.240	ml/mol	McGowan Method
rinpol	2237.00		NIST Webbook
rinpol	2266.00		NIST Webbook
tf	434.65	K	Aqueous Solubility Prediction Method
tf	433.05	K	The dissolution behaviour and apparent thermodynamic analysis of diprophylline in pure and mixed solvents

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	39.30	kJ/mol	435.70	NIST Webbook

Sources

Aqueous and cosolvent solubility data for drug-like organic compounds: https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C479185&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

The dissolution behaviour and apparent thermodynamic analysis of diprophylline in pure and mixed solvents: https://www.doi.org/10.1016/j.jct.2019.06.007

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

Legend

hfust:	Enthalpy of fusion at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point