Etofylline

Other names:	1,3-Dimethyl-7-(2-hydroxyethyl)xanthine
	1H-Purine-2,6-dione, 3,7-dihydro-7-(2-hydroxyethyl)-1,3-dimethyl-
	3,7-Dihydro-7-(2-hydroxyethyl)-1,3-dimethyl-1H-purine-2,6-dione
	7-(.beta.-hydroxyethyl)theophylline
	7-(2'-Hydroxyethyl)theophylline
	7-(2-hydroxyethyl)-1,3-dimethyl-3,7-dihydro-1H-purine-2,6-dione
	7-(2-hydroxyethyl)-1,3-dimethylxanthine
	7-(2-hydroxyethyl)theophylline
	7-(Hydroxyethyl)theophylline
	7-(«beta»-Hydroxyethyl)theophylline
	7-Theophyllineethanol
	Aethophyllinum
	Ascorphylline
	Bio-phylline
	Cordalin
	Corophyllin-N
	Dilaphyllin
	Frekaphyllin
	Hydroxyethyltheophylline
	NSC 113373
	OT
	Oxphylline
	Oxphylline (Amido)
	Oxyaethyltheophyllin
	Oxyethyltheophylline
	Oxyphylline
	Oxytheonyl
	Phyllocormin N
	Sklerodormal
	Soluphylline
	Theophylline, 2-hydroxyethyl
	Theophylline, 7-(2-hydroxyethyl)-
Inchi:	InChI=1S/C9H12N4O3/c1-11-7-6(8(15)12(2)9(11)16)13(3-4-14)5-10-7/h5,14H,3-4H2,1-2
InchiKey:	NWPRCRWQMGIBOT-UHFFFAOYSA-N
Formula:	C9H12N4O3
SMILES:	Cn1c(=O)c2c(ncn2CCO)n(C)c1=O
Mol. weight [g/mol]:	224.22
CAS:	519-37-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.99		Crippen Method
logp	-1.574		Crippen Method
mcvol	156.280	ml/mol	McGowan Method
rinpol	2090.00		NIST Webbook
tf	435.80	K	The physicochemical properties and solubility of pharmaceuticals - Methyl xanthines

Sources

The physicochemical properties and solubility of pharmaceuticals - Methyl xanthines:	https://www.doi.org/10.1016/j.jct.2014.05.005
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C519379&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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