Proxyphylline

Other names:	1H-Purine-2,6-dione, 3,7-dihydro-7-(2-hydroxypropyl)-1,3-dimethyl-
	Theophylline, 7-(2-hydroxypropyl)-
	«beta»-Hydroxypropyltheophylline
	Brontyl
	Hydroxypropyltheophylline
	Monophylline
	Oxypropyltheophylline
	Proxiphylline
	Purophyllin
	Sanwaphyllin
	Sigophyl
	Spasmolysin
	Thean
	Theoden
	1,3-Dimethyl-7-(2-hydroxypropyl)xanthine
	2-Hydroxypropyl-7-theophylline
	7-(«beta»-Hydroxypropyl)-1,3-dimethylxanthine
	7-(«beta»-Hydroxypropyl)theophylline
	7-(2-Hydroxypropyl)theophylline
	MT
	Proxy-Retardoral
	Theon
	1H-Purine-2,6-dione, 3,7-dihydro-1,3-dimethyl-7-(2-hydroxypropyl)-
	3,7-Dihydro-7-(2-hydroxypropyl)-1,3-dimethyl-1H-purine-2,6-dione
	Spantin
	NSC 163343
Inchi:	InChI=1S/C10H14N4O3/c1-6(15)4-14-5-11-8-7(14)9(16)13(3)10(17)12(8)2/h5-6,15H,4H2
InchiKey:	KYHQZNGJUGFTGR-UHFFFAOYSA-N
Formula:	C10H14N4O3
SMILES:	CC(O)Cn1cnc2c1c(=O)n(C)c(=O)n2C
Mol. weight [g/mol]:	238.24
CAS:	603-00-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.52		Crippen Method

logp	-1.186		Crippen Method
mcvol	170.370	ml/mol	McGowan Method
rinpol	2103.00		NIST Webbook

Sources

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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C603009&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices