Pentifylline

Other names:	1H-Purine-2,6-dione, 1-hexyl-3,7-dihydro-3,7-dimethyl-
	1H-Purine-2,6-dione, 3,7-dihydro-1-hexyl-3,7-dimethyl-
	Cosadon
	Cosaldon
	1-Hexyl-3,7-dimethylxanthine
	Hexyltheobromine
	1-Hexyltheobromine
	Pentifyllin
	SK 7
	Theobromine, 1-hexyl-
	1-Hexyl-3,7-dihydro-3,7-dimethyl-1H-purine-2,6-dione
	3,7-Dimethyl-1-hexyl-1H,3H-purin-2,6-dione
	SK 7 (pharmaceutical)
Inchi:	InChI=1S/C13H20N4O2/c1-4-5-6-7-8-17-12(18)10-11(14-9-15(10)2)16(3)13(17)19/h9H,4
InchiKey:	MRWQRJMESRRJJB-UHFFFAOYSA-N
Formula:	C13H20N4O2
SMILES:	CCCCCCn1c(=O)c2c(ncn2C)n(C)c1=O
Mol. weight [g/mol]:	264.32
CAS:	1028-33-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.40		Crippen Method
logp	1.014		Crippen Method
mcvol	206.770	ml/mol	McGowan Method
rinpol	2195.00		NIST Webbook
rinpol	2195.00		NIST Webbook
rinpol	2195.00		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

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices