

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:

CCCCCn1c(=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

Latest version available from:

<https://www.chemeo.com/cid/16-605-2/Pentifylline.pdf>

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