8-CHLOROTHEOPHYLLINE

Other names:	1H-Purine-2,6-dione, 8-chloro-3,7-dihydro-1,3-dimethyl- Theophylline, 8-chloro- 1,3-Dimethyl-8-chloroxanthine 8-Chlorotheophyline
Inchi:	InChI=1S/C7H7ClN4O2/c1-11-4-3(9-6(8)10-4)5(13)12(2)7(11)14/h1-2H3,(H,9,10)
InchiKey:	RYIGNEOBDRVTHA-UHFFFAOYSA-N
Formula:	C7H7ClN4O2
SMILES:	Cn1c(=O)c2[nH]c(Cl)nc2n(C)c1=O
Mol. weight [g/mol]:	214.61

Physical Properties

Property code	Value	Unit	Source
logp	-0.868		Crippen Method
mcvol	134.470	ml/mol	McGowan Method
tf	591.59	K	Cheméo Relay (1.0)

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C85187&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point