

1-Ethyltheobromine

Inchi:	InChI=1S/C9H12N4O2/c1-4-13-8(14)6-7(10-5-11(6)2)12(3)9(13)15/h5H,4H2,1-3H3
InchiKey:	KRVVZXPQPXJE-UHFFFAOYSA-N
Formula:	C9H12N4O2
SMILES:	CCn1c(=O)c2c(ncn2C)n(C)c1=O
Mol. weight [g/mol]:	208.22

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.72		Aqueous and cosolvent solubility data for drug-like organic compounds
logp	-0.546		Crippen Method
mcvol	150.410	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Aqueous and cosolvent solubility data for drug-like organic compounds:	https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/
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

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