

1-Butyltheobromine

Inchi:	InChI=1S/C11H16N4O2/c1-4-5-6-15-10(16)8-9(12-7-13(8)2)14(3)11(15)17/h7H,4-6H2,1-
InchiKey:	ZCUPBJOZMPROIJ-UHFFFAOYSA-N
Formula:	C11H16N4O2
SMILES:	CCCCn1c(=O)c2c(ncn2C)n(C)c1=O
Mol. weight [g/mol]:	236.28

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.62		Aqueous and cosolvent solubility data for drug-like organic compounds
logp	0.234		Crippen Method
mcvol	178.590	ml/mol	McGowan Method

Sources

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

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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