6-Azathymine, Bis(methyl) ether

Other names: 6-Azathymine, dimethyl ether
Inchi: InChI=1S/C6H9N3O2/c1-4-5(10-2)7-6(11-3)9-8-4/h1-3H3
InchiKey: PWRAMXNLJWGUOE-UHFFFAOYSA-N
Formula: C6H9N3O2
SMILES: COc1nnc(C)c(OC)n1
Mol. weight [g/mol]: 155.15

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.48		Crippen Method
logp	0.197		Crippen Method
mcvol	113.320	ml/mol	McGowan Method
rinpol	1262.20		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U333804&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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