

Purine, 7-benzyl-6-methoxy-

Inchi:	InChI=1S/C13H12N4O/c1-18-13-11-12(14-8-15-13)16-9-17(11)7-10-5-3-2-4-6-10/h2-6,8
InchiKey:	AQEQMZIQUIYEOE-UHFFFAOYSA-N
Formula:	C13H12N4O
SMILES:	COc1ncnc2ncn(Cc3ccccc3)c12
Mol. weight [g/mol]:	240.26
CAS:	21802-76-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.25		Crippen Method
logp	1.883		Crippen Method
mcvol	177.140	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C21802766&Units=SI

Legend

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

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<https://www.chemeo.com/cid/45-972-3/Purine-7-benzyl-6-methoxy.pdf>

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