

Purine, 2-amino-6-propoxy-

Inchi:	InChI=1S/C8H11N5O/c1-2-3-14-7-5-6(11-4-10-5)12-8(9)13-7/h4H,2-3H2,1H3,(H3,9,10,1
InchiKey:	WWMYHQCOEFJVFT-UHFFFAOYSA-N
Formula:	C8H11N5O
SMILES:	CCCOc1nc(N)nc2nc[nH]c12
Mol. weight [g/mol]:	193.21
CAS:	6331-91-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.38		Crippen Method
logp	0.242		Crippen Method
mcvol	140.430	ml/mol	McGowan Method

Sources

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=C6331915&Units=SI
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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<https://www.chemeo.com/cid/33-612-5/Purine-2-amino-6-propoxy.pdf>

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