

Purine, 6-propoxy-

Other names:	6-propoxy-1H-purine
Inchi:	InChI=1S/C8H10N4O/c1-2-3-13-8-6-7(10-4-9-6)11-5-12-8/h4-5H,2-3H2,1H3,(H,9,10,11,12)
InchiKey:	UQQKEKTYLCCYSN-UHFFFAOYSA-N
Formula:	C8H10N4O
SMILES:	CCCOc1ncnc2nc[nH]c12
Mol. weight [g/mol]:	178.19
CAS:	5417-86-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.75		Crippen Method
logp	0.660		Crippen Method
mcvol	130.450	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=C5417867&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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/18-128-0/Purine-6-propoxy.pdf>

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