

Purine, 6-propylthio-

Inchi:	InChI=1S/C8H10N4S/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:	BNLUVMLJJNTHSU-UHFFFAOYSA-N
Formula:	C8H10N4S
SMILES:	CCCSc1ncnc2[nH]cnc12
Mol. weight [g/mol]:	194.26
CAS:	6288-93-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.37		Crippen Method
logp	1.373		Crippen Method
mcvol	140.930	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6288933&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

Latest version available from:

<https://www.chemeo.com/cid/16-610-6/Purine-6-propylthio.pdf>

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