

6-(Octylthio)purine

Other names:	6-n-Octylmercaptapurine Purine, 6-(octylthio)- 1H-Purine, 6-(octylthio)- 7H-Purine, 6-(octylthio)-
Inchi:	InChI=1S/C13H20N4S/c1-2-3-4-5-6-7-8-18-13-11-12(15-9-14-11)16-10-17-13/h9-10H,2-
InchiKey:	YUEJEKKOQIRLNK-UHFFFAOYSA-N
Formula:	C13H20N4S
SMILES:	CCCCCCCCSc1ncnc2[nH]cnc12
Mol. weight [g/mol]:	264.39
CAS:	6974-89-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.47		Crippen Method
logp	3.324		Crippen Method
mcvol	211.380	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6974896&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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/83-227-8/6-Octylthio-purine.pdf>

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