

Purine, 6-(decylthio)-

Inchi:	InChI=1S/C15H24N4S/c1-2-3-4-5-6-7-8-9-10-20-15-13-14(17-11-16-13)18-12-19-15/h11
InchiKey:	IZEYPLNZOVRJBO-UHFFFAOYSA-N
Formula:	C15H24N4S
SMILES:	CCCCCCCCCSc1ncnc2nc[nH]c12
Mol. weight [g/mol]:	292.44
CAS:	6974-90-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.30		Crippen Method
logp	4.104		Crippen Method
mcvol	239.560	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6974909&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

Latest version available from:

<https://www.chemeo.com/cid/83-645-4/Purine-6-decylthio.pdf>

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