

Purine, 6-(ethylthio)-

Inchi:	InChI=1S/C7H8N4S/c1-2-12-7-5-6(9-3-8-5)10-4-11-7/h3-4H,2H2,1H3,(H,8,9,10,11)
InchiKey:	XTJLAIOQORFEOI-UHFFFAOYSA-N
Formula:	C7H8N4S
SMILES:	CCSc1ncnc2nc[nH]c12
Mol. weight [g/mol]:	180.23
CAS:	5417-84-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.95		Crippen Method
logp	0.983		Crippen Method
mvol	126.840	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=C5417845&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mvol:	McGowan's characteristic volume

Latest version available from:

<https://www.chemeo.com/cid/62-717-7/Purine-6-ethylthio.pdf>

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