

Purine, 8-(methylsulfonyl)-

Inchi:	InChI=1S/C6H6N4O2S/c1-13(11,12)6-9-4-2-7-3-8-5(4)10-6/h2-3H,1H3,(H,7,8,9,10)
InchiKey:	JVDLELCXTCJCSN-UHFFFAOYSA-N
Formula:	C6H6N4O2S
SMILES:	CS(=O)(=O)c1nc2ncncc2[nH]1
Mol. weight [g/mol]:	198.20
CAS:	10179-91-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.49		Crippen Method
logp	-0.726		Crippen Method
mcvol	124.490	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=C10179916&Units=SI

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/35-997-7/Purine-8-methylsulfonyl.pdf>

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