

Purine, 6-butylamino-2-methylthio-

Inchi:	InChI=1S/C10H15N5S/c1-3-4-5-11-8-7-9(13-6-12-7)15-10(14-8)16-2/h6H,3-5H2,1-2H3,(
InchiKey:	YEZACIOSMXFXIA-UHFFFAOYSA-N
Formula:	C10H15N5S
SMILES:	CCCCNc1nc(SC)nc2nc[nH]c12
Mol. weight [g/mol]:	237.32
CAS:	104294-77-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.80		Crippen Method
logp	1.805		Crippen Method
mcvol	179.090	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=C104294771&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
mcvol:	McGowan's characteristic volume

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<https://www.chemeo.com/cid/78-718-9/Purine-6-butylamino-2-methylthio.pdf>

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