

9H-purine, 2-amino-6-(butylamino)-

Inchi:	InChI=1S/C9H14N6/c1-2-3-4-11-7-6-8(13-5-12-6)15-9(10)14-7/h5H,2-4H2,1H3,(H4,10,11)
InchiKey:	REMXDSRYVGKQHF-UHFFFAOYSA-N
Formula:	C9H14N6
SMILES:	CCCCNc1nc(N)nc2[nH]cnc12
Mol. weight [g/mol]:	206.25
CAS:	5437-50-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.69		Crippen Method
logp	0.665		Crippen Method
mcvol	158.630	ml/mol	McGowan Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5437503&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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