

Purine, 2-(n-butylamino)-6-(dimethylamino)-

Inchi:	InChI=1S/C11H18N6/c1-4-5-6-12-11-15-9-8(13-7-14-9)10(16-11)17(2)3/h7H,4-6H2,1-3H
InchiKey:	JHXLGYKRRFKGGQ-UHFFFAOYSA-N
Formula:	C11H18N6
SMILES:	CCCCNc1nc(N(C)C)c2[nH]cnc2n1
Mol. weight [g/mol]:	234.30
CAS:	5463-10-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.97		Crippen Method
logp	1.149		Crippen Method
mcvol	186.810	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C5463105&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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