Purine, 2-amino-6-butoxy-

Inchi:	InChI=1S/C9H13N5O/c1-2-3-4-15-8-6-7(12-5-11-6)13-9(10)14-8/h5H,2-4H2,1H3,(H3,10,
InchiKey:	SPHOZXNZJHRHSL-UHFFFAOYSA-N
Formula:	C9H13N5O
SMILES:	CCCCOc1nc(N)nc2nc[nH]c12
Mol. weight [g/mol]:	207.23
CAS:	76412-62-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.80		Crippen Method
logp	0.632		Crippen Method
mcvol	154.520	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=C76412629&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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