

Guanine, 9-butyl-

Inchi:	InChI=1S/C9H13N5O/c1-2-3-4-14-5-11-6-7(14)12-9(10)13-8(6)15/h5H,2-4H2,1H3,(H3,10)
InchiKey:	RITMSEHRRVJGJR-UHFFFAOYSA-N
Formula:	C9H13N5O
SMILES:	CCCCn1cnc2c(=O)[nH]c(N)nc21
Mol. weight [g/mol]:	207.23
CAS:	93905-75-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.18		Crippen Method
logp	0.020		Crippen Method
mcvol	154.520	ml/mol	McGowan Method

Sources

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=C93905750&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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/45-009-2/Guanine-9-butyl.pdf>

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