

9H-purine, 9-butyl-

Inchi:	InChI=1S/C9H12N4/c1-2-3-4-13-7-12-8-5-10-6-11-9(8)13/h5-7H,2-4H2,1H3
InchiKey:	KXLZDRFOELIMKK-UHFFFAOYSA-N
Formula:	C9H12N4
SMILES:	CCCCn1cnc2cncnc21
Mol. weight [g/mol]:	176.22
CAS:	6943-34-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.67		Crippen Method
logp	1.626		Crippen Method
mcvol	138.670	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6943346&Units=SI
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

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/59-848-6/9H-purine-9-butyl.pdf>

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