

Hypoxanthine, 7-butyl-

Inchi:	InChI=1S/C9H12N4O/c1-2-3-4-6-12-7-8(13-6)10-5-11-9(7)14/h5H,2-4H2,1H3,(H2,10,11,
InchiKey:	ADFWGGCOWHEJLR-UHFFFAOYSA-N
Formula:	C9H12N4O
SMILES:	CCCCc1nc2nc[nH]c(=O)c2[nH]1
Mol. weight [g/mol]:	192.22

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.31		Crippen Method
logp	0.025		Crippen Method
mcvol	144.540	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=B6010452&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

Latest version available from:

<https://www.chemeo.com/cid/48-070-1/Hypoxanthine-7-butyl.pdf>

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