

Hypoxanthine, 1-butyl-

Inchi:	InChI=1S/C9H12N4O/c1-2-3-4-13-6-12-8-7(9(13)14)10-5-11-8/h5-6H,2-4H2,1H3,(H,10,1
InchiKey:	BNUMIKQQOKMWQA-UHFFFAOYSA-N
Formula:	C9H12N4O
SMILES:	CCCCn1cnc2[nH]cnc2c1=O
Mol. weight [g/mol]:	192.22
CAS:	40067-44-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.55		Crippen Method
logp	0.438		Crippen Method
mcvol	144.540	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=C40067445&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/40-396-8/Hypoxanthine-1-butyl.pdf>

Generated by Cheméo on 2025-12-06 00:20:56.270929773 +0000 UTC m=+4728653.800970427.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.