

9-Methylpoxanthine

Other names:	9-Methylhypoxanthine
Inchi:	InChI=1S/C6H6N4O/c1-10-3-9-4-5(10)7-2-8-6(4)11/h2-3H,1H3,(H,7,8,11)
InchiKey:	PESGUQRDJASXOR-UHFFFAOYSA-N
Formula:	C6H6N4O
SMILES:	Cn1cnc2c(O)ncnc21
Mol. weight [g/mol]:	150.14
CAS:	875-31-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.41		Crippen Method
logp	0.069		Crippen Method
mcvol	102.270	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=C875310&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

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