

Urea, 1-methyl, 3-[9h-purin-6-ylaminoethyl]-

Inchi:	InChI=1S/C9H13N7O/c1-10-9(17)12-3-2-11-7-6-8(14-4-13-6)16-5-15-7/h4-5H,2-3H2,1H3
InchiKey:	NQVXIIYBYMSBIH-UHFFFAOYSA-N
Formula:	C9H13N7O
SMILES:	CNC(=O)NCCNc1ncnc2[nH]cnc12
Mol. weight [g/mol]:	235.25
CAS:	7151-39-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.19		Crippen Method
logp	-0.788		Crippen Method
mcvol	170.180	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7151395&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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