

Urea, 1-methyl-3-(1,2,3,4-tetrahydro-2,4-dioxo-5-pyrimidinyl)-

Other names:	Urea, 1-(2,4-dihydroxy-5-pyrimidinyl)-3-methyl-
Inchi:	InChI=1S/C6H8N4O3/c1-7-5(12)9-3-2-8-6(13)10-4(3)11/h2H,1H3,(H2,7,9,12)(H2,8,10,11)
InchiKey:	LEWZDWLIXVPXRA-UHFFFAOYSA-N
Formula:	C6H8N4O3
SMILES:	CNC(=O)Nc1c[nH]c(=O)[nH]c1=O
Mol. weight [g/mol]:	184.15
CAS:	89533-45-9

Physical Properties

Property code	Value	Unit	Source
log10ws	0.88		Crippen Method
logp	-2.149		Crippen Method
mcvol	124.870	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C89533459&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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