Acetamide, 9h-purine-9-yl

Inchi:	InChI=1S/C7H7N5O/c8-6(13)2-12-4-11-5-1-9-3-10-7(5)12/h1,3-4H,2H2,(H2,8,13)
InchiKey:	QSRCCSWUFSZXJQ-UHFFFAOYSA-N
Formula:	C7H7N5O
SMILES:	NC(=O)Cn1cnc2cncnc21
Mol. weight [g/mol]:	177.16
CAS:	99595-72-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.04		Crippen Method
logp	-0.688		Crippen Method
mcvol	122.040	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=C99595729&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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/26-146-1/Acetamide-9h-purine-9-yl.pdf
Generated by Cheméo on 2024-10-12 08:32:27.294569707 +0000 UTC m=+3302809.931538955.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.