

N-1H-Tetrazol-5-ylacetamide

Other names:	Acetamide, N-1H-tetrazol-5-yl- 5-Acetamidotetrazole Tetrazole, 5-acetamido- NSC 402738
Inchi:	InChI=1S/C3H5N5O/c1-2(9)4-3-5-7-8-6-3/h1H3,(H2,4,5,6,7,8,9)
InchiKey:	JDVYHWSDERZPMV-UHFFFAOYSA-N
Formula:	C3H5N5O
SMILES:	CC(O)=Nc1nn[nH]n1
Mol. weight [g/mol]:	127.10
CAS:	6158-77-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.37		Crippen Method
logp	-0.674		Crippen Method
mvol	85.140	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6158776&Units=SI
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

Legend

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

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