

Oxamide, n-[3-(1-aziridiny)propyl]-

Inchi:	InChI=1S/C7H13N3O2/c8-6(11)7(12)9-2-1-3-10-4-5-10/h1-5H2,(H2,8,11)(H,9,12)
InchiKey:	NZNJMRUHUSZTRM-UHFFFAOYSA-N
Formula:	C7H13N3O2
SMILES:	NC(=O)C(=O)NCCCN1CC1
Mol. weight [g/mol]:	171.20
CAS:	24480-30-6

Physical Properties

Property code	Value	Unit	Source
log10ws	0.61		Crippen Method
logp	-1.706		Crippen Method
mcvol	131.710	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C24480306&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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