

1-Imidazolidinecarboxamide, n-(2-chloroethyl)-3-nitroso-2-oxo-

Inchi: InChI=1S/C6H9ClN4O3/c7-1-2-8-5(12)10-3-4-11(9-14)6(10)13/h1-4H2,(H,8,12)
InchiKey: MKAJQRIQIMGZQW-UHFFFAOYSA-N
Formula: C6H9ClN4O3
SMILES: O=NN1CCN(C(=O)NCCCCI)C1=O
Mol. weight [g/mol]: 220.61
CAS: 16813-34-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.40		Crippen Method
logp	0.354		Crippen Method
mcvol	141.410	ml/mol	McGowan Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C16813346&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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