1-Methoxy-2,2,3-trimethylaziridine (sin)

Other names: Aziridine, 1-methoxy-2,2,3-trimethyl, syn
Inchi: InChI=1S/C6H13NO/c1-5-6(2,3)7(5)8-4/h5H,1-4H3
InchiKey: VNGCQFBBUOYGPX-UHFFFAOYSA-N
Formula: C6H13NO
SMILES: CON1C(C)C1(C)C
Mol. weight [g/mol]: 115.17
CAS: 40802-08-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.10		Crippen Method
logp	1.030		Crippen Method
mcvol	100.390	ml/mol	McGowan Method
rinpol	725.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C40802082&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
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices