8-Azabicyclo[3.2.1]octane, 3-chloro-8-methyl-

Other names: 3-Chlorotropane
Inchi: InChI=1S/C8H14ClN/c1-10-7-2-3-8(10)5-6(9)4-7/h6-8H,2-5H2,1H3
InchiKey: WXRBWXUZUHYHQS-UHFFFAOYSA-N
Formula: C8H14ClN
SMILES: CN1C2CCC1CC(Cl)C2
Mol. weight [g/mol]: 159.66
CAS: 51275-31-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.02		Crippen Method
logp	1.850		Crippen Method
mcvol	124.080	ml/mol	McGowan Method
rinpol	1221.80		NIST Webbook
rinpol	1221.80		NIST Webbook

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=C51275311&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
rinpol: Non-polar retention indices

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