

3-Chloro-1-azabicyclo[2.2.2]octane

Inchi: InChI=1S/C7H12ClN/c8-7-5-9-3-1-6(7)2-4-9/h6-7H,1-5H2
InchiKey: NOLVABYTFMDREN-UHFFFAOYSA-N
Formula: C7H12ClN
SMILES: ClC1CN2CCCC1CC2
Mol. weight [g/mol]: 145.63
CAS: 42332-45-6

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| affp | 954.30 | kJ/mol | NIST Webbook |
| basg | 923.50 | kJ/mol | NIST Webbook |
| ie | 8.80 | eV | NIST Webbook |
| log10ws | -1.14 | | Crippen Method |
| logp | 1.319 | | Crippen Method |
| mcvol | 109.990 | ml/mol | McGowan Method |

Sources

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>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C42332456&Units=SI>

Legend

affp: Proton affinity
basg: Gas basicity
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

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