

8-Azabicyclo[3.2.1]octane,3-bromo-8-methyl-endo

Inchi: InChI=1S/C8H14BrN/c1-10-7-2-3-8(10)5-6(9)4-7/h6-8H,2-5H2,1H3
InchiKey: ASXOSTZMQJKYRY-UHFFFAOYSA-N
Formula: C8H14BrN
SMILES: CN1C2CCC1CC(Br)C2
Mol. weight [g/mol]: 204.11
CAS: 27809-79-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.30		Crippen Method
logp	2.006		Crippen Method
mcvol	129.340	ml/mol	McGowan Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C27809796&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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