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

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: 2292-11-7

Physical Properties

Property code	Value	Unit	Source
ie	7.80 ± 0.15	eV	NIST Webbook
log10ws	-2.30		Crippen Method
logp	2.006		Crippen Method
mcvol	129.340	ml/mol	McGowan Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2292117&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.