

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

Other names:	8-Azabicyclo[3.2.1]octane,3-chloro-8-methyl-endo-
Inchi:	InChI=1S/C8H14ClN/c1-10-7-2-3-8(10)5-6(9)4-7/h6-8H,2-5H2,1H3
InchiKey:	WXRWBWXUZYHYHQS-UHFFFAOYSA-N
Formula:	C8H14ClN
SMILES:	CN1C2CCC1CC(Cl)C2
Mol. weight [g/mol]:	159.66

Physical Properties

Property code	Value	Unit	Source
ie	8.10 ± 0.15	eV	NIST Webbook
logp	1.850		Crippen Method
mcvol	124.080	ml/mol	McGowan Method
tb	489.90	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C13514039&Units=SI>

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature

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