

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:	WXRWBWXUZYHYHQS-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

Latest version available from:

<https://www.chemeo.com/cid/81-385-5/8-Azabicyclo-3-2-1-octane-3-chloro-8-methyl.pdf>

Generated by Cheméo on 2025-12-05 14:01:21.56175262 +0000 UTC m=+4691479.091793285.

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