

Clomethiazole

Other names:	Thiazole, 5-(2-chloroethyl)-4-methyl- Chlorethiazol Chlorethiazole Chlormethiazol Chlormethiazole 5-(2-Chloroethyl)-4-methylthiazole Clomethiazolum Distraneurin Emineurina 4-Methyl-5-(«beta»-chloroethyl)thiazole Somnevrin WY 1485 Chloro-S.C.T.Z.
Inchi:	InChI=1S/C6H8CINS/c1-5-6(2-3-7)9-4-8-5/h4H,2-3H2,1H3
InchiKey:	PCLITLDTJTVDJ-UHFFFAOYSA-N
Formula:	C6H8CINS
SMILES:	Cc1ncsc1CCCl
Mol. weight [g/mol]:	161.65
CAS:	533-45-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.43		Crippen Method
logp	2.233		Crippen Method
mcvol	114.510	ml/mol	McGowan Method
rinpol	1221.00		NIST Webbook
rinpol	1221.00		NIST Webbook
rinpol	1228.00		NIST Webbook
rinpol	1235.00		NIST Webbook
rinpol	1230.00		NIST Webbook
rinpol	1245.00		NIST Webbook
rinpol	1240.00		NIST Webbook
rinpol	1230.00		NIST Webbook
rinpol	1230.00		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=C533459&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
rinpola:	Non-polar retention indices

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