

Methyclothiazide

Inchi:	InChI=1S/C9H11Cl2N3O4S2/c1-14-9(4-10)13-6-2-5(11)7(19(12,15)16)3-8(6)20(14,17)18
InchiKey:	CESYKOGBSMNBPD-UHFFFAOYSA-N
Formula:	C9H11Cl2N3O4S2
SMILES:	CN1C(CCl)Nc2cc(Cl)c(S(N)(=O)=O)cc2S1(=O)=O
Mol. weight [g/mol]:	360.24
CAS:	135-07-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.71		Cheméo Relay (1.0)
logp	0.598		Crippen Method
mcvol	213.650	ml/mol	McGowan Method
tf	498.15	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Jean-Claude Bradley Open Melting
Point Dataset (2014, CC0):
McGowan Method:

https://figshare.com/articles/Jean_Claude_Bradley_Open_Melting_Point_Dataset/1031637

<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

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point

Latest version available from:

<https://www.chemeo.com/cid/112-085-3/Methyclothiazide.pdf>

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