Clomethiazole M (di-OH)

Inchi: InChI=1S/C6H8ClNO2S/c7-1-5(10)6-4(2-9)8-3-11-6/h3,5,9-10H,1-2H2
InchiKey: UGBYDXPYTGNTTI-UHFFFAOYSA-N
Formula: C6H8ClNO2S
SMILES: OCc1ncsc1C(O)CCl
Mol. weight [g/mol]: 193.65

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.82		Crippen Method
logp	0.908		Crippen Method
mcvol	126.250	ml/mol	McGowan Method
rinpol	1590.00		NIST Webbook
rinpol	1590.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=R57377&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

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