N-(2-mercaptoethyl)-1,3-thiazolidine

Inchi: InChI=1S/C5H11NS2/c7-3-1-6-2-4-8-5-6/h7H,1-5H2
InchiKey: QZSFSYKRUWBUHJ-UHFFFAOYSA-N
Formula: C5H11NS2
SMILES: SCCN1CCSC1
Mol. weight [g/mol]: 149.28

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.83		Crippen Method
logp	0.923		Crippen Method
mcvol	113.130	ml/mol	McGowan Method
rinpol	1325.00		NIST Webbook
rinpol	1325.00		NIST Webbook
ripol	2035.00		NIST Webbook
ripol	2035.00		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=R239284&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
ripol: Polar retention indices