

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/ci9903071>

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

Latest version available from:

<https://www.cheméo.com/cid/63-380-0/N-2-mercaptoethyl-1-3-thiazolidine.pdf>

Generated by Cheméo on 2024-04-29 01:53:42.846271745 +0000 UTC m=+16644871.766849056.

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