

N-Carboxyethylrhodanine

Other names:	3-Thiazolidinepropanoic acid, 4-oxo-2-thioxo-3-Thiazolidinepropionic acid, 4-oxo-2-thioxo-4-Oxo-2-thioxo-3-thiazolidinepropionic acid Rhodanine-3-propionic acid Rodanin-3-propionic acid 4-oxo-2-thioxothiazolidine-3-propionic acid
Inchi:	InChI=1S/C6H7NO3S2/c8-4-3-12-6(11)7(4)2-1-5(9)10/h1-3H2,(H,9,10)
InchiKey:	SWAHCTPCIUXXTQ-UHFFFAOYSA-N
Formula:	C6H7NO3S2
SMILES:	O=C(O)CCN1C(=O)CSC1=S
Mol. weight [g/mol]:	205.25
CAS:	7025-19-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.90		Crippen Method
logp	0.321		Crippen Method
mcvol	131.930	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7025196&Units=SI
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

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