Alanine, n,n'-(dithiodiethylene)di-

Inchi:	InChI=1S/C10H20N2O4S2/c1-7(9(13)14)11-3-5-17-18-6-4-12-8(2)10(15)16/h7-8,11-12H
InchiKey:	PQYZJHWCCCXNSM-UHFFFAOYSA-N
Formula:	C10H20N2O4S2
SMILES:	CC([NH2+]CCSSCC[NH2+]C(C)C(=O)[O-])C(=O)[O-]
Mol. weight [g/mol]:	296.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.34		Crippen Method
logp	-4.229		Crippen Method
mcvol	219.300	ml/mol	McGowan Method

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=B6009914&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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