

4-(N-butylsulfonylmethyl)-4-thiazoline-2-thione

Inchi:	InChI=1S/C8H13NO2S3/c1-2-3-4-14(10,11)6-7-5-13-8(12)9-7/h5H,2-4,6H2,1H3,(H,9,12)
InchiKey:	ZDJKPMShPGTQTD-UHFFFAOYSA-N
Formula:	C8H13NO2S3
SMILES:	CCCCS(=O)(=O)Cc1csc(=S)[nH]1
Mol. weight [g/mol]:	251.39
CAS:	90087-94-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.69		Crippen Method
logp	2.039		Crippen Method
mcvol	174.890	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C90087948&Units=SI
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

Legend

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

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