

3-Anilinorhodanine

Other names:	4-Thiazolidinone, 3-(phenylamino)-2-thioxo-Thiazolidin-4-one, 3-phenylamino-2-thioxo-
Inchi:	InChI=1S/C9H8N2OS2/c12-8-6-14-9(13)11(8)10-7-4-2-1-3-5-7/h1-5,10H,6H2
InchiKey:	SNRGCDPTDOAQEQ-UHFFFAOYSA-N
Formula:	C9H8N2OS2
SMILES:	O=C1CSC(=S)N1Nc1ccccc1
Mol. weight [g/mol]:	224.30
CAS:	13097-10-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.78		Crippen Method
logp	1.874		Crippen Method
mcvol	152.980	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13097104&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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