

4-Thiazolidinone, 3-phenyl-2-thioxo-

Other names:	N-Phenylrhodanine Rhodanine, 3-phenyl- 3-Phenylrhodanin 3-Phenylrhodanine 3-Phenylrodanin 3-Phenyl-2-thioxo-1,3-thiazolidin-4-one NSC 17528 3-Phenylrhodanide
Inchi:	InChI=1S/C9H7NOS2/c11-8-6-13-9(12)10(8)7-4-2-1-3-5-7/h1-5H,6H2
InchiKey:	DVRWEKGUWZINTQ-UHFFFAOYSA-N
Formula:	C9H7NOS2
SMILES:	O=C1CSC(=S)N1c1ccccc1
Mol. weight [g/mol]:	209.29
CAS:	1457-46-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.70		Crippen Method
logp	2.051		Crippen Method
mcvol	143.000	ml/mol	McGowan Method

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=C1457461&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

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