

Rhodanine, 5-cyclohexylidene-3-phenyl

Inchi:	InChI=1S/C15H15NOS2/c17-14-13(11-7-3-1-4-8-11)19-15(18)16(14)12-9-5-2-6-10-12/h2
InchiKey:	OLTSSWCGWALRTA-UHFFFAOYSA-N
Formula:	C15H15NOS2
SMILES:	O=C1C(=C2CCCCC2)SC(=S)N1c1ccccc1
Mol. weight [g/mol]:	289.42
CAS:	35610-74-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.45		Crippen Method
logp	4.269		Crippen Method
mcvol	212.380	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=C35610743&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

Latest version available from:

<https://www.chemeo.com/cid/84-849-7/Rhodanine-5-cyclohexylidene-3-phenyl.pdf>

Generated by Cheméo on 2024-05-03 03:53:16.754751576 +0000 UTC m=+16997645.675328891.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.