Rhodanine, 5-(p-dimethylaminobenzylidene)-3-(p-dimethylami

Inchi:	InChI=1S/C21H22N4OS2/c1-23(2)17-9-5-15(6-10-17)13-19-20(26)25(21(27)28-19)22-14
InchiKey:	TWESMUXYFSDURT-QTLAEQSKSA-N
Formula:	C21H22N4OS2
SMILES:	CN(C)c1ccc(C=NN2C(=O)C(=Cc3ccc(N(C)C)cc3)SC2=S)cc1
Mol. weight [g/mol]:	410.56
CAS:	35532-35-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.20		Crippen Method
logp	4.054		Crippen Method
mcvol	309.660	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C35532355&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

Latest version available from:
https://www.chemeo.com/cid/46-847-1/Rhodanine-5-p-dimethylaminobenzylidene-3-p-dimethylaminobenzylideneami
Generated by Cheméo on 2024-05-05 18:30:23.875749387 +0000 UTC m=+17223072.796326703.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.