

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

Inchi:	InChI=1S/C18H16N2OS2/c1-19(2)14-10-8-13(9-11-14)12-16-17(21)20(18(22)23-16)15-6
InchiKey:	JOYWVNFXPQUIAZ-FOWTUZBSSA-N
Formula:	C18H16N2OS2
SMILES:	CN(C)c1ccc(C=C2SC(=S)N(c3ccccc3)C2=O)cc1
Mol. weight [g/mol]:	340.46
CAS:	3698-12-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.16		Crippen Method
logp	4.158		Crippen Method
mcvol	251.730	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C3698122&Units=SI

Legend

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

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