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/ci990307l

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