

Rhodanine, 5-(p-methoxybenzylidene)-3-(p-methoxybenzylideneamino)-

Inchi: InChI=1S/C19H16N2O3S2/c1-23-15-7-3-13(4-8-15)11-17-18(22)21(19(25)26-17)20-12-13
InchiKey: IJYFZVKHEOGKFS-WYRLOYKNSA-N
Formula: C19H16N2O3S2
SMILES: COc1ccc(C=NN2C(=O)C(=Cc3ccc(OC)cc3)SC2=S)cc1
Mol. weight [g/mol]: 384.47
CAS: 94258-53-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.63		Crippen Method
logp	3.939		Crippen Method
mcvol	273.260	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=C94258534&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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