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

Inchi: InChI=1S/C19H16N2O3S2/c1-23-15-7-3-13(4-8-15)11-17-18(22)21(19(25)26-17)20-12-1

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