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

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=C35532355&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume