Rhodanine, 5-benzylidene-3-phenyl

Inchi: InChI=1S/C16H11NOS2/c18-15-14(11-12-7-3-1-4-8-12)20-16(19)17(15)13-9-5-2-6-10-13
InchiKey: TZPSGDWUSVAMNF-SDNWHVSQSA-N
Formula: C16H11NOS2
SMILES: O=C1C(=Cc2ccccc2)SC(=S)N1c1ccccc1
Mol. weight [g/mol]: 297.39
CAS: 13037-56-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.25		Crippen Method
logp	4.092		Crippen Method
mcvol	213.570	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=C13037564&Units=SI

Legend

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