

Rhodanine, 5-(p-chlorobenzylidene)-3-(p-chlorobenzylideneamino)

Inchi:	InChI=1S/C17H10Cl2N2OS2/c18-13-5-1-11(2-6-13)9-15-16(22)21(17(23)24-15)20-10-12
InchiKey:	WDEDNBRHAZYXPU-SABIUBGXSA-N
Formula:	C17H10Cl2N2OS2
SMILES:	O=C1C(=Cc2ccc(Cl)cc2)SC(=S)N1N=Cc1ccc(Cl)cc1
Mol. weight [g/mol]:	393.31
CAS:	17521-25-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.76		Crippen Method
logp	5.229		Crippen Method
mcvol	257.820	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=C17521254&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

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