2-Benzothiazolinethione, 3-(o-chloroanilinomethyl)-

Inchi: InChI=1S/C14H11ClN2S2/c15-10-5-1-2-6-11(10)16-9-17-12-7-3-4-8-13(12)19-14(17)18/h

InchiKey: GSMFTTGTJYKLEN-UHFFFAOYSA-N

Formula: C14H11ClN2S2

SMILES: S=c1sc2ccccc2n1CNc1ccccc1Cl

Mol. weight [g/mol]: 306.83

CAS: 116400-95-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.15		Crippen Method
logp	5.155		Crippen Method
mcvol	210.340	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C116400954&Units=SI

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

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume