

10-(N-octadecyl)phenothiazine

Inchi:	InChI=1S/C30H45NS/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-21-26-31-27-22-17-19-20
InchiKey:	IGUHKPOQPVTBEO-UHFFFAOYSA-N
Formula:	C30H45NS
SMILES:	CCCCCCCCCCCCCCCCCN1c2ccccc2Sc2ccccc21
Mol. weight [g/mol]:	451.75
CAS:	16262-72-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-10.95		Crippen Method
logp	10.551		Crippen Method
mcvol	401.510	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=C16262729&Units=SI

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/64-705-8/10-N-octadecyl-phenothiazine.pdf>

Generated by Cheméo on 2024-04-19 15:29:07.099367375 +0000 UTC m=+15829796.019944688.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.