

Benzo[b]phenanthro[3,2-d]thiophene, 13-methyl

Inchi:	InChI=1S/C21H14S/c1-13-20-15(11-10-14-6-2-3-7-16(14)20)12-19-21(13)17-8-4-5-9-18(
InchiKey:	XKKTZRYTVDHXDG-UHFFFAOYSA-N
Formula:	C21H14S
SMILES:	Cc1c2c(ccc3ccccc32)cc2sc3ccccc3c12
Mol. weight [g/mol]:	298.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.92		Crippen Method
logp	6.669		Crippen Method
mcvol	225.800	ml/mol	McGowan Method
rinpola	511.19		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R21354&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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
rinpola:	Non-polar retention indices

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