

Benzo[2,3]phenanthro[4,5]thiophene, 3-methyl

Inchi:	InChI=1S/C19H12S/c1-11-6-9-16-18-14(11)8-7-13-10-12-4-2-3-5-15(12)19(20-16)17(13)
InchiKey:	ZPUMKGGXGJGWZFS-UHFFFAOYSA-N
Formula:	C19H12S
SMILES:	Cc1ccc2sc3c4ccccc4cc4ccc1c2c43
Mol. weight [g/mol]:	272.36

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.34		Crippen Method
logp	6.107		Crippen Method
mcvol	201.920	ml/mol	McGowan Method
rinpol	461.10		NIST Webbook

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=R642501&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

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