

acenaphtho[4,3-b]benzo[d]thiophene

Inchi:	InChI=1S/C18H12S/c1-2-7-15-13(6-1)18-14-9-8-11-4-3-5-12(17(11)14)10-16(18)19-15/h
InchiKey:	JKSVSYMOAXIDQO-UHFFFAOYSA-N
Formula:	C18H12S
SMILES:	c1cc2c3c(c4c(cc3c1)sc1cccc14)CC2
Mol. weight [g/mol]:	260.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.31		Crippen Method
logp	5.306		Crippen Method
mcvol	192.130	ml/mol	McGowan Method
rinpola	456.18		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R197690&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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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