benzo[2,3]fluorantheno[1,12-bcd]thiophene

Inchi:	InChI=1S/C20H10S/c1-2-6-15-11(5-1)12-7-3-8-13-14-9-4-10-16-18(14)19(17(12)13)20(1
InchiKey:	QYYUKRSTVJRPNA-UHFFFAOYSA-N
Formula:	C20H10S
SMILES:	c1cc2c3c(c1)sc1c4ccccc4c4cccc-2c4c13
Mol. weight [g/mol]:	282.36

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.30		Crippen Method
logp	6.341		Crippen Method
mcvol	200.850	ml/mol	McGowan Method
rinpol	507.50		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R197709&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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