Dinaphtho[1,2-b:1',2'-d]thiophene

Other names:	dinaphtho[1,1-b:1',2'-d]thiophene
	dinaphto[1,2-b:1',2'-d]thiophene
	Dinaphtho[1,2-b;1',2'-d]thiophene
Inchi:	InChI=1S/C20H12S/c1-3-7-15-13(5-1)10-12-18-19(15)17-11-9-14-6-2-4-8-16(14)20(17)2
InchiKey:	SYXXZXWLYNODHL-UHFFFAOYSA-N
Formula:	C20H12S
SMILES:	c1ccc2c(c1)ccc1c2sc2ccc3ccccc3c21
Mol. weight [g/mol]:	284.37
CAS:	207-94-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.45		Crippen Method
logp	6.361		Crippen Method
mcvol	211.710	ml/mol	McGowan Method
rinpol	484.60		NIST Webbook
rinpol	486.58		NIST Webbook
rinpol	472.89		NIST Webbook
rinpol	479.70		NIST Webbook
rinpol	479.10		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C207943&Units=SI
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

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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