

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

Other names:	Naphtho(2,1-b)naphtho(1,2-d)thiophene Dinaphtho[2,1-b;1',2'-d]thiophene
Inchi:	InChI=1S/C20H12S/c1-3-7-15-13(5-1)9-11-17-19(15)20-16-8-4-2-6-14(16)10-12-18(20)2
InchiKey:	JFNCOYXPHARAMI-UHFFFAOYSA-N
Formula:	C20H12S
SMILES:	c1ccc2c(c1)ccc1sc3ccc4ccccc4c3c12
Mol. weight [g/mol]:	284.37
CAS:	194-65-0

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	470.00		NIST Webbook
rinpol	472.62		NIST Webbook
rinpol	461.20		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C194650&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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