

Naphtho[2,1-b]thiophene

Other names:	Naphtho[2.1-b]thiophene
Inchi:	InChI=1S/C12H8S/c1-2-4-10-9(3-1)5-6-12-11(10)7-8-13-12/h1-8H
InchiKey:	LJOLGGXHRVADAA-UHFFFAOYSA-N
Formula:	C12H8S
SMILES:	<chem>c1ccc2c(c1)ccc1sccc12</chem>
Mol. weight [g/mol]:	184.26
CAS:	233-02-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.84		Crippen Method
logp	4.054		Crippen Method
mcvol	137.910	ml/mol	McGowan Method
rinpol	300.00		NIST Webbook
rinpol	300.31		NIST Webbook
rinpol	300.00		NIST Webbook
rinpol	299.03		NIST Webbook
rinpol	299.79		NIST Webbook
rinpol	300.00		NIST Webbook
rinpol	299.41		NIST Webbook
rinpol	300.00		NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C233023&Units=SI

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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