

Naphtho[1,2-b]thiophene

Other names:	6,7-Benzothionaphthene
Inchi:	InChI=1S/C12H8S/c1-2-4-11-9(3-1)5-6-10-7-8-13-12(10)11/h1-8H
InchiKey:	XHYRHAQEXJIVJX-UHFFFAOYSA-N
Formula:	C12H8S
SMILES:	<chem>c1ccc2c(c1)ccc1ccsc12</chem>
Mol. weight [g/mol]:	184.26
CAS:	234-41-3

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	295.52		NIST Webbook
rinpol	295.80		NIST Webbook
rinpol	294.26		NIST Webbook
rinpol	293.28		NIST Webbook
rinpol	292.86		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C234413&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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