

Naphtho[2,3-b]thiophene

Other names:	Naphtha[2,3-b]thiophene thiaphanthrene thiophanthrene
Inchi:	InChI=1S/C12H8S/c1-2-4-10-8-12-11(5-6-13-12)7-9(10)3-1/h1-8H
InchiKey:	CYKIHIBNSFRKQP-UHFFFAOYSA-N
Formula:	C12H8S
SMILES:	c1ccc2cc3sccc3cc2c1
Mol. weight [g/mol]:	184.26
CAS:	268-77-9

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	304.28		NIST Webbook
rinpol	304.10		NIST Webbook
rinpol	304.46		NIST Webbook
rinpol	304.47		NIST Webbook
rinpol	304.56		NIST Webbook
rinpol	304.10		NIST Webbook
rinpol	304.28		NIST Webbook
rinpol	303.56		NIST Webbook
rinpol	304.33		NIST Webbook
rinpol	304.28		NIST Webbook
tf	461.70	K	Reconciled thermophysical data for anthracene

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C268779&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Reconciled thermophysical data for anthracene:	https://www.doi.org/10.1016/j.jct.2018.08.034

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpola:	Non-polar retention indices
tf:	Normal melting (fusion) point

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