

Benzo[b]naphtho[2,3-d]thiophene

Other names:	Benzo[b]naphto[2,3-d]thiophene Benzo[b]naphtho[2,3]thiophene Benzo[a]naphtho[2,3-d]thiophene
Inchi:	InChI=1S/C16H10S/c1-2-6-12-10-16-14(9-11(12)5-1)13-7-3-4-8-15(13)17-16/h1-10H
InchiKey:	UWMISBRPSJFHIR-UHFFFAOYSA-N
Formula:	C16H10S
SMILES:	<chem>c1ccc2cc3c(cc2c1)sc1cccc13</chem>
Mol. weight [g/mol]:	234.32
CAS:	243-46-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.64		Crippen Method
logp	5.208		Crippen Method
mcvol	174.810	ml/mol	McGowan Method
rinpol	395.20		NIST Webbook
rinpol	395.90		NIST Webbook
rinpol	395.60		NIST Webbook
rinpol	395.59		NIST Webbook
rinpol	395.79		NIST Webbook
rinpol	395.61		NIST Webbook
rinpol	395.97		NIST Webbook
rinpol	394.76		NIST Webbook
rinpol	359.59		NIST Webbook
rinpol	395.59		NIST Webbook
rinpol	395.61		NIST Webbook
rinpol	395.50		NIST Webbook
rinpol	393.59		NIST Webbook
rinpol	395.20		NIST Webbook
rinpol	395.69		NIST Webbook
rinpol	395.70		NIST Webbook
rinpol	395.40		NIST Webbook
rinpol	395.20		NIST Webbook
rinpol	393.17		NIST Webbook
rinpol	395.76		NIST Webbook
rinpol	394.76		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C243469&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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