

Benzo[b]naphtho[1,2-d]thiophene

Other names:	Naphtho[2,1-b]thianaphthene 3,4-Benzo-9-thiafluorene 7-Thia-7H-benzo[c]fluorene Benzo[b]naphto[1,2-d]thiophene Benzo[b]naphtho[1,2]thiophene Dibenzo[b]naphtho[1,2d]thiopnene
Inchi:	InChI=1S/C16H10S/c1-2-6-12-11(5-1)9-10-15-16(12)13-7-3-4-8-14(13)17-15/h1-10H
InchiKey:	XZUMOEVHCZXMTR-UHFFFAOYSA-N
Formula:	C16H10S
SMILES:	<chem>c1ccc2c(c1)ccc1sc3ccccc3c12</chem>
Mol. weight [g/mol]:	234.32
CAS:	205-43-6

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	392.88		NIST Webbook
rinpol	392.70		NIST Webbook
rinpol	392.00		NIST Webbook
rinpol	2446.00		NIST Webbook
rinpol	2446.00		NIST Webbook
rinpol	392.94		NIST Webbook
rinpol	392.51		NIST Webbook
rinpol	392.24		NIST Webbook
rinpol	392.60		NIST Webbook
rinpol	395.00		NIST Webbook
rinpol	392.51		NIST Webbook
rinpol	393.73		NIST Webbook
rinpol	391.73		NIST Webbook
rinpol	392.59		NIST Webbook
rinpol	392.92		NIST Webbook
rinpol	391.73		NIST Webbook
rinpol	391.73		NIST Webbook
rinpol	392.51		NIST Webbook
rinpol	392.59		NIST Webbook

rinpol	390.69	NIST Webbook
rinpol	392.70	NIST Webbook
rinpol	391.47	NIST Webbook
rinpol	392.20	NIST Webbook
rinpol	392.18	NIST Webbook
rinpol	392.40	NIST Webbook
rinpol	392.00	NIST Webbook
rinpol	392.20	NIST Webbook
rinpol	390.33	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	19.00	kJ/mol	375.50	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=C205436&Units=SI

Legend

hfust:	Enthalpy of fusion at a given temperature
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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