

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

Other names:	Benzo[a]dibenzothiophene Naphtho[1,2-b]thianaphthene 1,2-Benzo-9-thiafluorene 1,2-Benzodiphenylene sulfide Benzo[b]naphtho[2,1]thiophene benzo[b]naphto[2,1-d]thiophene 11-thiabenzo[a]fluorene
Inchi:	InChI=1S/C16H10S/c1-2-6-12-11(5-1)9-10-14-13-7-3-4-8-15(13)17-16(12)14/h1-10H
InchiKey:	YEUHHUCOSQOCIX-UHFFFAOYSA-N
Formula:	C16H10S
SMILES:	c1ccc2c(c1)ccc1c3ccccc3sc21
Mol. weight [g/mol]:	234.32
CAS:	239-35-0

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	2333.00		NIST Webbook
rinpol	389.16		NIST Webbook
rinpol	389.04		NIST Webbook
rinpol	389.64		NIST Webbook
rinpol	389.40		NIST Webbook
rinpol	389.98		NIST Webbook
rinpol	389.13		NIST Webbook
rinpol	389.30		NIST Webbook
rinpol	389.30		NIST Webbook
rinpol	389.16		NIST Webbook
rinpol	389.21		NIST Webbook
rinpol	389.26		NIST Webbook
rinpol	389.40		NIST Webbook
rinpol	389.53		NIST Webbook
rinpol	388.64		NIST Webbook
rinpol	389.09		NIST Webbook
rinpol	389.16		NIST Webbook
rinpol	387.30		NIST Webbook

rinpol	389.40	NIST Webbook
rinpol	388.12	NIST Webbook
rinpol	388.70	NIST Webbook
rinpol	388.86	NIST Webbook
rinpol	388.90	NIST Webbook
rinpol	388.40	NIST Webbook
rinpol	388.70	NIST Webbook
rinpol	389.51	NIST Webbook
rinpol	389.37	NIST Webbook
rinpol	387.08	NIST Webbook
rinpol	388.05	NIST Webbook
rinpol	388.64	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	111.90 ± 1.20	kJ/mol	349.00	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=C239350&Units=SI

Legend

hsubt:	Enthalpy of sublimation 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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