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: c1ccc2cc3c(cc2c1)sc1ccccc13
Mol. weight [g/mol]: 234.32

Physical Properties

Property code	Value	Unit	Source
hf	301.60	kJ/mol	Cheméo Relay (1.0)
hvap	106.94	kJ/mol	Cheméo Relay (1.0)
ie	7.29	eV	Cheméo Relay (1.0)
log10ws	-7.26		Cheméo Relay (1.0)
logp	5.208		Crippen Method
mcvol	174.810	ml/mol	McGowan Method
pc	2746.34	kPa	Cheméo Relay (1.0, beta)
rinpol	394.76		NIST Webbook
rinpol	395.20		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	395.76		NIST Webbook
rinpol	395.61		NIST Webbook
rinpol	395.50		NIST Webbook
rinpol	393.59		NIST Webbook
rinpol	395.90		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	395.20		NIST Webbook
rinpol	395.59		NIST Webbook
tb	706.74	K	Cheméo Relay (1.0)
tc	990.89	K	Cheméo Relay (1.0)
tf	484.18	K	Cheméo Relay (1.0)
vc	0.664	m3/kmol	Cheméo Relay (1.0)

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C243469&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

hf: Enthalpy of formation at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume