

2,8-DIMETHYLDIBENZO(B,D)THIOPHENE

Other names:	2,8-Dimethyldibenzothiophene Dibenzothiophene, 2,8-dimethyl-
Inchi:	InChI=1S/C14H12S/c1-9-3-5-13-11(7-9)12-8-10(2)4-6-14(12)15-13/h3-8H,1-2H3
InchiKey:	RRYWCJRYULRSJM-UHFFFAOYSA-N
Formula:	C14H12S
SMILES:	Cc1ccc2sc3ccc(C)cc3c2c1
Mol. weight [g/mol]:	212.32

Physical Properties

Property code	Value	Unit	Source
af	0.4917		Cheméo Relay (1.0)
hf	155.28	kJ/mol	Cheméo Relay (1.0)
ie	7.47	eV	Cheméo Relay (1.0)
log10ws	-6.35		Cheméo Relay (1.0)
logp	4.671		Crippen Method
mcvol	166.090	ml/mol	McGowan Method
pc	2590.91	kPa	Cheméo Relay (1.0, beta)
rinpol	1947.00		NIST Webbook
rinpol	335.20		NIST Webbook
rinpol	335.80		NIST Webbook
rinpol	1947.00		NIST Webbook
rinpol	334.19		NIST Webbook
rinpol	332.00		NIST Webbook
rinpol	333.19		NIST Webbook
rinpol	335.90		NIST Webbook
rinpol	334.66		NIST Webbook
rinpol	335.80		NIST Webbook
rinpol	335.10		NIST Webbook
tb	638.73	K	Cheméo Relay (1.0)
tc	881.27	K	Cheméo Relay (1.0)
tf	441.20	K	Cheméo Relay (1.0)
vc	0.626	m3/kmol	Cheméo Relay (1.0)

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C1207154&Units=SI

Legend

af:	Acentric Factor
hf:	Enthalpy of formation 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

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