

Benzo[b]naphtho[2,3-d]thiophene, 6-methyl-

Other names:	6-Methylnaphtho[2,3-b][1]benzothiophene Benzo[b]naphtho[2,3]thiophene, 6-methyl 6-Methylbenzo(b)naphtho(2,3-d)thiophene Benzo[b]naphtho[2,1-d]thiophene, 2-methyl
Inchi:	InChI=1S/C17H12S/c1-11-13-7-3-2-6-12(13)10-15-14-8-4-5-9-16(14)18-17(11)15/h2-10H
InchiKey:	SMVYLXVOJHVADR-UHFFFAOYSA-N
Formula:	C17H12S
SMILES:	Cc1c2ccccc2cc2c1sc1cccc12
Mol. weight [g/mol]:	248.34
CAS:	24360-63-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.12		Crippen Method
logp	5.516		Crippen Method
mcvol	188.900	ml/mol	McGowan Method
rinpol	405.60		NIST Webbook
rinpol	413.05		NIST Webbook
rinpol	407.63		NIST Webbook
rinpol	415.02		NIST Webbook
rinpol	414.01		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=C24360632&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcpol: McGowan's characteristic volume
rinpol: Non-polar retention indices

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