

2,3,6-trimethyl-benzothiophene

Other names:	2,3,6-trimethyl-benzothiophene
Inchi:	InChI=1S/C11H12S/c1-7-4-5-10-8(2)9(3)12-11(10)6-7/h4-6H,1-3H3
InchiKey:	NETYMFPERAKHQJ-UHFFFAOYSA-N
Formula:	C11H12S
SMILES:	<chem>Cc1ccc2c(C)c(C)sc2c1</chem>
Mol. weight [g/mol]:	176.28

Physical Properties

Property code	Value	Unit	Source
hf	93.48	kJ/mol	Cheméo Relay (1.0)
ie	7.60	eV	Cheméo Relay (1.0)
logp	3.827		Crippen Method
mcvol	143.280	ml/mol	McGowan Method
tf	335.84	K	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=R85992&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
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point

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