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: Cc1ccc2c(C)c(C)sc2c1
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