THIOPHENE, 3,4-DIETHYL-

Inchi: InChI=1S/C8H12S/c1-3-7-5-9-6-8(7)4-2/h5-6H,3-4H2,1-2H3
InchiKey: KWMRVTDUWMBHRV-UHFFFAOYSA-N
Formula: C8H12S
SMILES: CCc1cscc1CC
Mol. weight [g/mol]: 140.25

Physical Properties

Property code	Value	Unit	Source
af	0.3757		Cheméo Relay (1.0)
hvap	49.66	kJ/mol	Cheméo Relay (1.0)
ie	8.30	eV	Cheméo Relay (1.0)
log10ws	-3.94		Cheméo Relay (1.0)
logp	2.873		Crippen Method
mcvol	120.470	ml/mol	McGowan Method
pc	3065.38	kPa	Cheméo Relay (1.0, beta)
tb	459.16	K	Cheméo Relay (1.0)
tc	665.17	K	Cheméo Relay (1.0)
tf	223.90	K	Cheméo Relay (1.0)
vc	0.438	m3/kmol	Cheméo Relay (1.0)

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C35686147&Units=SI
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):

Legend

af:	Acentric Factor
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume