2-(2-THIENYLTHIO)THIOPHENE

Other names: 2-(2-Thienylthio)thiophene
Inchi: InChI=1S/C8H6S3/c1-3-7(9-5-1)11-8-4-2-6-10-8/h1-6H
InchiKey: AKYIWBKPINOXJY-UHFFFAOYSA-N
Formula: C8H6S3
SMILES: c1csc(Sc2cccs2)c1
Mol. weight [g/mol]: 198.34

Physical Properties

Property code	Value	Unit	Source
hf	256.25	kJ/mol	Cheméo Relay (1.0)
hvap	71.71	kJ/mol	Cheméo Relay (1.0)
ie	8.40	eV	NIST Webbook
logp	3.961		Crippen Method
mcvol	133.710	ml/mol	McGowan Method
pc	4442.59	kPa	Cheméo Relay (1.0, beta)
tb	547.84	K	Cheméo Relay (1.0)
tc	779.25	K	Cheméo Relay (1.0)
tf	320.21	K	Cheméo Relay (1.0)
vc	0.470	m3/kmol	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3988996&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):

Legend

hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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