2,3-Dihydrothiophene 1,1-dioxide

Other names:	Thiophene, 2,3-dihydro-, 1,1-dioxide
	Sulfol-2-ene
	«alpha»-Sulfolene
	2-Sulfolene
Inchi:	InChI=1S/C4H6O2S/c5-7(6)3-1-2-4-7/h1,3H,2,4H2
InchiKey:	DYGJDTCGUUMUBL-UHFFFAOYSA-N
Formula:	C4H6O2S
SMILES:	O=S1(=O)C=CCC1
Mol. weight [g/mol]:	118.15
CAS:	1192-16-1

Physical Properties

Property code	Value	Unit	Source
chs	-2710.40 ± 1.60	kJ/mol	NIST Webbook
gf	-404.78	kJ/mol	Joback Method
hf	-262.00 ± 3.10	kJ/mol	NIST Webbook
hfs	-323.20 ± 1.70	kJ/mol	NIST Webbook
hfus	11.11	kJ/mol	Joback Method
hsub	61.50	kJ/mol	NIST Webbook
hvap	42.99	kJ/mol	Joback Method
ie	10.28	eV	NIST Webbook
ie	10.28	eV	NIST Webbook
ie	10.00	eV	NIST Webbook
log10ws	-0.57		Crippen Method
logp	0.319		Crippen Method
mcvol	80.150	ml/mol	McGowan Method
pc	6707.62	kPa	Joback Method
tb	336.86	K	Joback Method
tc	523.01	K	Joback Method
tf	238.35	K	Joback Method
vc	0.305	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	120.43	J/mol×K	336.86	Joback Method
cpg	130.30	J/mol×K	367.88	Joback Method
cpg	139.66	J/mol×K	398.91	Joback Method
cpg	148.52	J/mol×K	429.93	Joback Method
cpg	156.90	J/mol×K	460.96	Joback Method
cpg	164.80	J/mol×K	491.98	Joback Method
cpg	172.25	J/mol×K	523.01	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1192161&Units=SI

Legend

chs: Standard solid enthalpy of combustion
cpg: Ideal gas heat capacity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfs: Solid phase enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hsub: Enthalpy of sublimation at standard conditions
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