2,5-Dihydrothiophene sulfone

Other names:	1,1-DIOXIDE-2,5-DIHYDROTHIOPHENE
	2,5-Dihydrothiophene 1,1-dioxide
	2,5-Dihydrothiophene S,S-dioxide
	2,5-Dihydrothiophene dioxide
	3-Sulfolene
	BUTADIENE SULFONE
	NCI-C04557
	NSC 48532
	Sulfol-3-ene
	Sulfolene
	Sulpholene
	Thiophene, 2,5-dihydro-, 1,1-dioxide
	«beta»-Sulfolene
	Â«betaÂ»-Sulfolene
Inchi:	InChI=1S/C4H6O2S/c5-7(6)3-1-2-4-7/h1-2H,3-4H2
InchiKey:	MBDNRNMVTZADMQ-UHFFFAOYSA-N
Formula:	C4H6O2S
SMILES:	O=S1(=O)CC=CC1
Mol. weight [g/mol]:	118.15
CAS:	77-79-2

Physical Properties

Property code	Value	Unit	Source
gf	-404.78	kJ/mol	Joback Method
hf	-255.60 ± 1.70	kJ/mol	NIST Webbook
hfs	-318.40 ± 1.70	kJ/mol	NIST Webbook
hfus	11.11	kJ/mol	Joback Method
hsub	62.80	kJ/mol	NIST Webbook
hvap	42.99	kJ/mol	Joback Method
ie	10.00	eV	NIST Webbook
ie	10.44	eV	NIST Webbook
ie	10.35	eV	NIST Webbook
ie	10.44	eV	NIST Webbook
log10ws	-0.08		Crippen Method
logp	-0.029		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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C77792&Units=SI
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
KDB: https://www.cheric.org/files/research/kdb/mol/mol1866.mol
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

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