2,5-Dihydrothiophene 1,1-dioxide

Other names:	1,1-DIOXIDE-2,5-DIHYDROTHIOPHENE
	2,5-Dihydrothiophene S,S-dioxide
	2,5-Dihydrothiophene dioxide
	2,5-Dihydrothiophene sulfone
	3-Sulfolene
	BUTADIENE SULFONE
	NCI-C04557
	NSC 48532
	Sulfol-3-ene
	Sulfolene
	Sulpholene
	Thiophene, 2,5-dihydro-, 1,1-dioxide
	«beta»-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:	28452-93-9

Physical Properties

Property code	Value	Unit	Source
chs	-2714.90 ± 1.30	kJ/mol	NIST Webbook
hf	-256.20 ± 2.80	kJ/mol	NIST Webbook
hfs	-318.90 ± 1.30	kJ/mol	NIST Webbook
hfus	11.11	kJ/mol	Joback Method
ie	10.42	eV	Cheméo Relay (1.0)
logp	-0.029		Crippen Method
mcvol	80.150	ml/mol	McGowan 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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

KDB: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1866

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C28452939&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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

Legend

chs: Standard solid enthalpy of combustion

cpg: Ideal gas heat capacity

hf: Enthalpy of formation at standard conditions

hfs: Solid phase enthalpy of formation at standard conditions

hfus: Enthalpy of fusion at standard conditions

ie: Ionization energy

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume