

2,5-Dihydro-3-methyl-thiophene 1,1-dioxide

Other names:	3-Methylsulfolene Thiophene, 2,5-dihydro-3-methyl-, 1,1-dioxide 1,3-Butadiene, 2-methyl-, sulfone 3-Methyl-2,5-dihydrothiophene dioxide 3-Methyl-2,5-dihydrothiophene 1,1-dioxide 3-Methyl-3-sulfolene 2,5-Dihydrothiophene, 1,1-dioxide, 3-methyl- NSC 15090
Inchi:	InChI=1S/C5H8O2S/c1-5-2-3-8(6,7)4-5/h2H,3-4H2,1H3
InchiKey:	FAYFWMOSHFCQPG-UHFFFAOYSA-N
Formula:	C5H8O2S
SMILES:	CC1=CCS(=O)(=O)C1
Mol. weight [g/mol]:	132.18
CAS:	1193-10-8

Physical Properties

Property code	Value	Unit	Source
chs	-3357.40 ± 2.10	kJ/mol	NIST Webbook
gf	-405.99	kJ/mol	Joback Method
hf	-291.60 ± 2.20	kJ/mol	NIST Webbook
hfs	-355.60 ± 2.20	kJ/mol	NIST Webbook
hfus	13.31	kJ/mol	Joback Method
hsub	64.00	kJ/mol	NIST Webbook
hvap	45.87	kJ/mol	Joback Method
ie	9.84	eV	NIST Webbook
log10ws	-0.50		Crippen Method
logp	0.361		Crippen Method
mcvol	94.240	ml/mol	McGowan Method
pc	5636.27	kPa	Joback Method
tb	364.72	K	Joback Method
tc	552.22	K	Joback Method
tf	262.14	K	Joback Method
vc	0.361	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	156.71	J/mol×K	364.72	Joback Method
cpg	167.43	J/mol×K	395.97	Joback Method
cpg	177.62	J/mol×K	427.22	Joback Method
cpg	187.32	J/mol×K	458.47	Joback Method
cpg	196.53	J/mol×K	489.72	Joback Method
cpg	205.26	J/mol×K	520.97	Joback Method
cpg	213.53	J/mol×K	552.22	Joback Method

Sources

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=C1193108&Units=SI
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
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

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