

Thiophene, tetrahydro-3-methyl-, 1,1-dioxide

Other names:	3-METHYL SULFOLANE 3-Methylsulfolane 3-Methyltetrahydrothiophene 1,1-dioxide 3-Methylthiacyclopentane 1,1-dioxide
Inchi:	InChI=1S/C5H10O2S/c1-5-2-3-8(6,7)4-5/h5H,2-4H2,1H3
InchiKey:	CMJLMPKFQPJDKP-UHFFFAOYSA-N
Formula:	C5H10O2S
SMILES:	CC1CCS(=O)(=O)C1
Mol. weight [g/mol]:	134.20
CAS:	872-93-5

Physical Properties

Property code	Value	Unit	Source
gf	-434.03	kJ/mol	Joback Method
hf	-536.01	kJ/mol	Joback Method
hfus	13.55	kJ/mol	Joback Method
hvap	44.61	kJ/mol	Joback Method
log10ws	-0.40		Crippen Method
logp	0.441		Crippen Method
mcvol	98.540	ml/mol	McGowan Method
pc	5205.63	kPa	Joback Method
tb	550.00 ± 3.00	K	NIST Webbook
tc	539.07	K	Joback Method
tf	305.00 ± 0.80	K	NIST Webbook
vc	0.374	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	165.71	J/mol×K	355.91	Joback Method
cpg	178.40	J/mol×K	386.44	Joback Method
cpg	190.52	J/mol×K	416.96	Joback Method
cpg	202.11	J/mol×K	447.49	Joback Method
cpg	213.15	J/mol×K	478.02	Joback Method

cpg	223.68	J/mol×K	508.54	Joback Method
cpg	233.69	J/mol×K	539.07	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
Coeff. A	7.83891e+01
Coeff. B	-1.06964e+04
Coeff. C	-8.71418e+00
Coeff. D	2.19994e-06
Temperature range (K), min.	273.65
Temperature range (K), max.	817.00

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=C872935&Units=SI
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1875

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure

pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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