3-Methyl sulfolane

Other names:	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
hfus	13.55	kJ/mol	Joback Method
logp	0.441		Crippen Method
mcvol	98.540	ml/mol	McGowan Method
tb	550.00 ± 3.00	K	NIST Webbook
tf	305.00 ± 0.80	K	NIST Webbook

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(Pvp) = A + B/T + C*ln(T) + D*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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C872935&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

cpg: Ideal gas heat capacity
hfus: Enthalpy of fusion at standard conditions
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pvap: Vapor pressure
tb: Normal Boiling Point Temperature
tf: Normal melting (fusion) point