Propane, 1-(methylsulfinyl)-

Other names: Methyl propyl sulfoxide
Inchi: InChI=1S/C4H10OS/c1-3-4-6(2)5/h3-4H2,1-2H3
InchiKey: WOBARLJSXVAEGX-UHFFFAOYSA-N
Formula: C4H10OS
SMILES: CCCS(C)=O
Mol. weight [g/mol]: 106.19
CAS: 14094-08-7

Physical Properties

Property code	Value	Unit	Source
gf	-234.91	kJ/mol	Joback Method
hf	-331.63	kJ/mol	Joback Method
hfus	13.87	kJ/mol	Joback Method
hvap	37.22	kJ/mol	Joback Method
log10ws	-0.13		Crippen Method
logp	0.775		Crippen Method
mcvol	89.440	ml/mol	McGowan Method
pc	4351.13	kPa	Joback Method
rinpol	818.00		NIST Webbook
tb	349.20	K	Joback Method
tc	525.53	K	Joback Method
tf	171.32	K	Joback Method
vc	0.349	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	147.03	J/mol×K	349.20	Joback Method
cpg	155.60	J/mol×K	378.59	Joback Method
cpg	163.91	J/mol×K	407.98	Joback Method
cpg	171.96	J/mol×K	437.36	Joback Method
cpg	179.75	J/mol×K	466.75	Joback Method
cpg	187.27	J/mol×K	496.14	Joback Method
cpg	194.52	J/mol×K	525.53	Joback Method

Sources

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=C14094087&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume