Butane, 1-(methylsulfinyl)-

Other names:	Sulfoxide, butyl methyl
	Butyl methyl sulfoxide
	Methyl n-butyl sulfoxide
Inchi:	InChI=1S/C5H12OS/c1-3-4-5-7(2)6/h3-5H2,1-2H3
InchiKey:	QPKGDTBMWSPKDT-UHFFFAOYSA-N
Formula:	C5H12OS
SMILES:	CCCCS(C)=O
Mol. weight [g/mol]:	120.21
CAS:	2976-98-9

Physical Properties

Property code	Value	Unit	Source
gf	-226.49	kJ/mol	Joback Method
hf	-352.27	kJ/mol	Joback Method
hfus	16.46	kJ/mol	Joback Method
hvap	39.45	kJ/mol	Joback Method
log10ws	-0.55		Crippen Method
logp	1.165		Crippen Method
mcvol	103.530	ml/mol	McGowan Method
pc	3848.31	kPa	Joback Method
tb	372.08	K	Joback Method
tc	548.09	K	Joback Method
tf	182.59	K	Joback Method
vc	0.406	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	181.25	J/mol×K	372.08	Joback Method
cpg	191.31	J/mol×K	401.41	Joback Method
cpg	201.04	J/mol×K	430.75	Joback Method
cpg	210.45	J/mol×K	460.08	Joback Method
cpg	219.52	J/mol×K	489.42	Joback Method
cpg	228.27	J/mol×K	518.75	Joback Method

cpg	236.69	J/mol×K	548.09	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2976989&Units=SI
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

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