

# tert-Butyl methyl sulfoxide

<b>Inchi:</b>	InChI=1S/C5H12OS/c1-5(2,3)7(4)6/h1-4H3
<b>InchiKey:</b>	YPRPSRLQZMDWFO-UHFFFAOYSA-N
<b>Formula:</b>	C5H12OS
<b>SMILES:</b>	CS(=O)C(C)(C)C
<b>Mol. weight [g/mol]:</b>	120.21
<b>CAS:</b>	14094-11-2

## Physical Properties

Property code	Value	Unit	Source
gf	-223.65	kJ/mol	Joback Method
hf	-361.02	kJ/mol	Joback Method
hfus	9.05	kJ/mol	Joback Method
hvap	38.15	kJ/mol	Joback Method
log10ws	-0.66		Crippen Method
logp	1.163		Crippen Method
mcvol	103.530	ml/mol	McGowan Method
pc	3940.66	kPa	Joback Method
tb	368.85	K	Joback Method
tc	557.01	K	Joback Method
tf	185.01	K	Joback Method
vc	0.395	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	182.30	J/molxK	368.85	Joback Method
cpg	193.88	J/molxK	400.21	Joback Method
cpg	204.93	J/molxK	431.57	Joback Method
cpg	215.44	J/molxK	462.93	Joback Method
cpg	225.43	J/molxK	494.29	Joback Method
cpg	234.92	J/molxK	525.65	Joback Method
cpg	243.92	J/molxK	557.01	Joback Method

# Sources

<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C14094112&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C14094112&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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