tert-Butyl methyl sulfoxide

Inchi:	InChI=1S/C5H12OS/c1-5(2,3)7(4)6/h1-4H3
InchiKey:	YPRPSRLQZMDWFO-UHFFFAOYSA-N
Formula:	C5H12OS
SMILES:	CS(=O)C(C)(C)C
Mol. weight [g/mol]:	120.21
CAS:	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/mol×K	368.85	Joback Method
cpg	193.88	J/mol×K	400.21	Joback Method
cpg	204.93	J/mol×K	431.57	Joback Method
cpg	215.44	J/mol×K	462.93	Joback Method
cpg	225.43	J/mol×K	494.29	Joback Method
cpg	234.92	J/mol×K	525.65	Joback Method
cpg	243.92	J/mol×K	557.01	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C14094112&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

Latest version available from:

https://www.chemeo.com/cid/53-049-9/tert-Butyl-methyl-sulfoxide.pdf

Generated by Cheméo on 2024-10-12 08:15:23.72570755 +0000 UTC m=+3301786.362676797.

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.