Trimethylsulfonylmethane

Inchi: InChI=1S/C4H10O6S3/c1-11(5,6)4(12(2,7)8)13(3,9)10/h4H,1-3H3
InchiKey: QYBXIUDBUIUBHS-UHFFFAOYSA-N
Formula: C4H10O6S3
SMILES: CS(=O)(=O)C(S(C)(=O)=O)S(C)(=O)=O
Mol. weight [g/mol]: 250.31
CAS: 67294-81-9

Physical Properties

Property code	Value	Unit	Source
gf	-1425.26	kJ/mol	Joback Method
hf	-1491.22	kJ/mol	Joback Method
hfus	36.73	kJ/mol	Joback Method
hvap	80.02	kJ/mol	Joback Method
log10ws	0.90		Crippen Method
logp	-1.596		Crippen Method
mcvol	151.490	ml/mol	McGowan Method
pc	7845.35	kPa	Joback Method
ss	304.60	J/mol×K	NIST Webbook
tb	433.82	K	Joback Method
tc	598.03	K	Joback Method
tf	235.52	K	Joback Method
vc	0.631	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	348.59	J/mol×K	570.66	Joback Method
cpg	297.51	J/mol×K	433.82	Joback Method
cpg	308.40	J/mol×K	461.19	Joback Method
cpg	318.97	J/mol×K	488.56	Joback Method
cpg	329.21	J/mol×K	515.92	Joback Method
cpg	339.08	J/mol×K	543.29	Joback Method
cpg	357.70	J/mol×K	598.03	Joback Method
cps	269.62	J/mol×K	298.15	NIST Webbook

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=C67294819&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
cps:	Solid phase 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
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume