Methanesulfonylacetonitrile

Other names:	Methylsulfonylacetonitrile Acetonitrile, (methylsulfonyl)- mesylacetonitrile
Inchi:	InChI=1S/C3H5NO2S/c1-7(5,6)3-2-4/h3H2,1H3
InchiKey:	FOTRKCAZUSJCQD-UHFFFAOYSA-N
Formula:	C3H5NO2S
SMILES:	CS(=O)(=O)CC#N
Mol. weight [g/mol]:	119.14
CAS:	2274-42-2

Physical Properties

Property code	Value	Unit	Source
gf	-360.98	kJ/mol	Joback Method
hf	-393.72	kJ/mol	Joback Method
hfus	16.41	kJ/mol	Joback Method
hvap	51.39	kJ/mol	Joback Method
log10ws	0.22		Crippen Method
logp	-0.445		Crippen Method
mcvol	82.600	ml/mol	McGowan Method
pc	5281.57	kPa	Joback Method
tb	417.90	K	Joback Method
tc	607.73	K	Joback Method
tf	227.12	K	Joback Method
vc	0.355	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	147.13	J/mol×K	417.90	Joback Method
cpg	153.29	J/mol×K	449.54	Joback Method
cpg	159.24	J/mol×K	481.18	Joback Method
cpg	164.98	J/mol×K	512.82	Joback Method
cpg	170.49	J/mol×K	544.46	Joback Method
cpg	175.77	J/mol×K	576.09	Joback Method

cpg	180.81	J/mol×K	607.73	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2274422&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