Sulfurous acid, bis(1-methylethyl) ester

Other names:	Sulfurous acid, diisopropyl ester
	Diisopropyl sulfite
	Diisopropyl ester of sulphurous acid
Inchi:	InChI=1S/C6H14O3S/c1-5(2)8-10(7)9-6(3)4/h5-6H,1-4H3
InchiKey:	IIKLEMKAKOISSP-UHFFFAOYSA-N
Formula:	C6H14O3S
SMILES:	CC(C)OS(=O)OC(C)C
Mol. weight [g/mol]:	166.24
CAS:	4773-13-1

Physical Properties

Property code	Value	Unit	Source
gf	-432.95	kJ/mol	Joback Method
hf	-647.91	kJ/mol	Joback Method
hfus	14.38	kJ/mol	Joback Method
hvap	45.72	kJ/mol	Joback Method
log10ws	-1.35		Crippen Method
logp	1.415		Crippen Method
mcvol	129.360	ml/mol	McGowan Method
pc	3356.75	kPa	Joback Method
tb	438.92	K	Joback Method
tc	622.07	K	Joback Method
tf	208.32	K	Joback Method
vc	0.485	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	264.55	J/mol×K	438.92	Joback Method
cpg	276.24	J/mol×K	469.44	Joback Method
cpg	287.61	J/mol×K	499.97	Joback Method
cpg	298.66	J/mol×K	530.49	Joback Method
cpg	309.35	J/mol×K	561.02	Joback Method
cpg	319.69	J/mol×K	591.54	Joback Method

cpg	329.64	J/mol×K	622.07	Joback Method

Sources

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=C4773131&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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