Acetic acid, trifluoro-, 2,2,2-trifluoro-1-methyl-1-(trifluoromethyl)ethyl ester

Othernames: Trifluoroacetic acid, 2,2,2-trifluoro-1-methyl-1-(trifluoromethyl)ethyl ester
Inchi: InChI=1S/C6H3F9O2/c1-3(5(10,11)12,6(13,14)15)17-2(16)4(7,8)9/h1H3
InchiKey: QKFTWDCMJRDXJG-UHFFFAOYSA-N
Formula: C6H3F9O2
SMILES: CC(OC(=O)C(F)(F)F)(C(F)(F)F)C(F)(F)F
Mol. weight [g/mol]: 278.07
CAS: 42031-16-3

Physical Properties

Property code	Value	Unit	Source
gf	-1976.21	kJ/mol	Joback Method
hf	-2211.96	kJ/mol	Joback Method
hfus	12.15	kJ/mol	Joback Method
hvap	25.57	kJ/mol	Joback Method
log10ws	-3.30		Crippen Method
logp	2.975		Crippen Method
mcvol	118.770	ml/mol	McGowan Method
pc	2318.07	kPa	Joback Method
tb	393.48	K	Joback Method
tc	535.72	K	Joback Method
tf	244.53	K	Joback Method
vc	0.513	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	327.05	J/mol×K	512.01	Joback Method
cpg	281.26	J/mol×K	393.48	Joback Method
cpg	291.69	J/mol×K	417.19	Joback Method
cpg	301.46	J/mol×K	440.89	Joback Method
cpg	310.59	J/mol×K	464.60	Joback Method
cpg	319.11	J/mol×K	488.30	Joback Method
cpg	334.44	J/mol×K	535.72	Joback Method
hvapt	33.50	kJ/mol	338.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C42031163&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
hvapt:	Enthalpy of vaporization at a given temperature
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