Acetic acid, trifluoro-, 2,2-dimethylpropyl ester

Other names: Trifluoroacetic acid, 2,2-dimethylpropyl ester
Inchi: InChI=1S/C7H11F3O2/c1-6(2,3)4-12-5(11)7(8,9)10/h4H2,1-3H3
InchiKey: FWFLFZDXCNIPGS-UHFFFAOYSA-N
Formula: C7H11F3O2
SMILES: CC(C)(C)COC(=O)C(F)(F)F
Mol. weight [g/mol]: 184.16
CAS: 7556-79-8

Physical Properties

Property code	Value	Unit	Source
gf	-804.61	kJ/mol	Joback Method
hf	-1038.44	kJ/mol	Joback Method
hfus	11.08	kJ/mol	Joback Method
hvap	35.29	kJ/mol	Joback Method
log10ws	-2.04		Crippen Method
logp	2.138		Crippen Method
mcvol	122.240	ml/mol	McGowan Method
pc	2654.29	kPa	Joback Method
tb	427.20	K	Joback Method
tc	597.87	K	Joback Method
tf	247.42	K	Joback Method
vc	0.483	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	268.09	J/mol×K	427.20	Joback Method
cpg	279.92	J/mol×K	455.65	Joback Method
cpg	291.12	J/mol×K	484.09	Joback Method
cpg	301.72	J/mol×K	512.54	Joback Method
cpg	311.73	J/mol×K	540.98	Joback Method
cpg	321.18	J/mol×K	569.43	Joback Method
cpg	330.10	J/mol×K	597.87	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=C7556798&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