Glycine, N-trifluoroacetyl-, isopropyl ester

Other names:	Glycine, N-trifluoroacetyl, 1-methylethyl ester
	Glycine, trifluoroacetyl, isopropyl ester
Inchi:	InChI=1S/C7H10F3NO3/c1-4(2)14-5(12)3-11-6(13)7(8,9)10/h4H,3H2,1-2H3,(H,11,13)
InchiKey:	NMMHHNLBWAZRMW-UHFFFAOYSA-N
Formula:	C7H10F3NO3
SMILES:	CC(C)OC(=O)CNC(=O)C(F)(F)F
Mol. weight [g/mol]:	213.15
CAS:	56936-67-5

Physical Properties

Property code	Value	Unit	Source
gf	-849.42	kJ/mol	Joback Method
hf	-1094.08	kJ/mol	Joback Method
hfus	21.67	kJ/mol	Joback Method
hvap	49.38	kJ/mol	Joback Method
log10ws	-1.35		Crippen Method
logp	0.617		Crippen Method
mcvol	133.790	ml/mol	McGowan Method
pc	2841.41	kPa	Joback Method
tb	534.03	K	Joback Method
tc	711.18	K	Joback Method
tf	332.59	K	Joback Method
vc	0.529	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	328.73	J/mol×K	534.03	Joback Method
cpg	339.15	J/mol×K	563.55	Joback Method
cpg	349.03	J/mol×K	593.08	Joback Method
cpg	358.36	J/mol×K	622.60	Joback Method
cpg	367.18	J/mol×K	652.13	Joback Method
cpg	375.49	J/mol×K	681.65	Joback Method
cpg	383.31	J/mol×K	711.18	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=C56936675&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