Glycine, N-[N-(trifluoroacetyl)glycyl]-, methyl ester

Other names: Trifluoroacetylglycylglycine methyl ester
N-[N-(Trifluoroacetyl)glycyl]glycine methyl ester
Inchi: InChI=1S/C7H9F3N2O4/c1-16-5(14)3-11-4(13)2-12-6(15)7(8,9)10/h2-3H2,1H3,(H,11,13)
InchiKey: VQFVYTURUFTZIM-UHFFFAOYSA-N
Formula: C7H9F3N2O4
SMILES: COC(=O)CNC(=O)CNC(=O)C(F)(F)F
Mol. weight [g/mol]: 242.15
CAS: 433-33-0

Physical Properties

Property code	Value	Unit	Source
gf	-886.51	kJ/mol	Joback Method
hf	-1147.91	kJ/mol	Joback Method
hfus	31.89	kJ/mol	Joback Method
hvap	62.95	kJ/mol	Joback Method
log10ws	-0.21		Crippen Method
logp	-1.046		Crippen Method
mcvol	145.340	ml/mol	McGowan Method
pc	3059.17	kPa	Joback Method
tb	638.51	K	Joback Method
tc	822.31	K	Joback Method
tf	450.18	K	Joback Method
vc	0.577	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	387.63	J/mol×K	638.51	Joback Method
cpg	396.79	J/mol×K	669.14	Joback Method
cpg	405.37	J/mol×K	699.78	Joback Method
cpg	413.38	J/mol×K	730.41	Joback Method
cpg	420.86	J/mol×K	761.04	Joback Method
cpg	427.81	J/mol×K	791.67	Joback Method
cpg	434.25	J/mol×K	822.31	Joback Method

hsubt	127.90	kJ/mol	371.00	NIST Webbook
hvapt	93.80	kJ/mol	431.50	NIST Webbook

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C433330&Units=SI

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
hsubt:	Enthalpy of sublimation at a given temperature
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