

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

Other names:	N-[N-(N-[trifluoroacetyl]glycyl)glycyl]glycine methyl ester
Inchi:	InChI=1S/C9H12F3N3O5/c1-20-7(18)4-14-5(16)2-13-6(17)3-15-8(19)9(10,11)12/h2-4H2
InchiKey:	JRPDARCFVAMKNG-UHFFFAOYSA-N
Formula:	C9H12F3N3O5
SMILES:	COC(=O)CN=C(O)CN=C(O)CN=C(O)C(F)(F)F
Mol. weight [g/mol]:	299.20
CAS:	651-18-3

Physical Properties

Property code	Value	Unit	Source
hf	-1310.37	kJ/mol	Joback Method
hvap	101.26	kJ/mol	Joback Method
log10ws	-0.06		Crippen Method
logp	0.591		Crippen Method
mcvol	185.070	ml/mol	McGowan Method
pc	2111.94	kPa	Joback Method
tb	982.41	K	Joback Method
tc	1203.17	K	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	133.40	kJ/mol	388.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C651183&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

hf:	Enthalpy of formation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
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

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