

Glycine, N-(trifluoroacetyl)-, methyl ester

Other names:	Methyl [(trifluoroacetyl)amino]acetate
Inchi:	InChI=1S/C5H6F3NO3/c1-12-3(10)2-9-4(11)5(6,7)8/h2H2,1H3,(H,9,11)
InchiKey:	BTZLVUPFAOBHFS-UHFFFAOYSA-N
Formula:	C5H6F3NO3
SMILES:	COC(=O)CNC(=O)C(F)(F)F
Mol. weight [g/mol]:	185.10
CAS:	383-72-2

Physical Properties

Property code	Value	Unit	Source
gf	-863.82	kJ/mol	Joback Method
hf	-1047.52	kJ/mol	Joback Method
hfus	20.02	kJ/mol	Joback Method
hvap	45.31	kJ/mol	Joback Method
log10ws	-0.41		Crippen Method
logp	-0.162		Crippen Method
mcvol	105.610	ml/mol	McGowan Method
pc	3493.01	kPa	Joback Method
rinpol	955.00		NIST Webbook
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tb	488.71	K	Joback Method
tc	665.53	K	Joback Method
tf	325.05	K	Joback Method
vc	0.423	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	243.40	J/molxK	488.71	Joback Method
cpg	251.71	J/molxK	518.18	Joback Method
cpg	259.57	J/molxK	547.65	Joback Method
cpg	267.01	J/molxK	577.12	Joback Method
cpg	274.03	J/molxK	606.59	Joback Method
cpg	280.64	J/molxK	636.06	Joback Method

cpg	286.86	J/mol×K	665.53	Joback Method
hsubt	57.30	kJ/mol	378.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C383722&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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