N-Trifluoroacetyl glycine

Other names: N-(Trifluoroacetyl)aminoacetic acid
Inchi: InChI=1S/C4H4F3NO3/c5-4(6,7)3(11)8-1-2(9)10/h1H2,(H,8,11)(H,9,10)
InchiKey: IFAXXCBMQJNCCF-UHFFFAOYSA-N
Formula: C4H4F3NO3
SMILES: O=C(O)CNC(=O)C(F)(F)F
Mol. weight [g/mol]: 171.07
CAS: 383-70-0

Physical Properties

Property code	Value	Unit	Source
gf	-904.06	kJ/mol	Joback Method
hf	-1046.89	kJ/mol	Joback Method
hfus	20.33	kJ/mol	Joback Method
hvap	57.36	kJ/mol	Joback Method
log10ws	-0.22		Crippen Method
logp	-0.250		Crippen Method
mcvol	91.520	ml/mol	McGowan Method
pc	4522.49	kPa	Joback Method
tb	535.59	K	Joback Method
tc	707.26	K	Joback Method
tf	352.37	K	Joback Method
vc	0.368	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	221.42	J/mol×K	535.59	Joback Method
cpg	227.50	J/mol×K	564.20	Joback Method
cpg	233.20	J/mol×K	592.81	Joback Method
cpg	238.52	J/mol×K	621.43	Joback Method
cpg	243.47	J/mol×K	650.04	Joback Method
cpg	248.09	J/mol×K	678.65	Joback Method
cpg	252.39	J/mol×K	707.26	Joback Method
hsubt	98.80	kJ/mol	333.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C383700&Units=SI
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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume