N-[N-(Trifluoroacetyl)glycylglycine

Inchi: InChI=1S/C6H7F3N2O4/c7-6(8,9)5(15)11-1-3(12)10-2-4(13)14/h1-2H2,(H,10,12)(H,11,15
InchiKey: UWXMXPPHLZYYPM-UHFFFAOYSA-N
Formula: C6H7F3N2O4
SMILES: O=C(O)CNC(=O)CNC(=O)C(F)(F)F
Mol. weight [g/mol]: 228.13
CAS: 400-58-8

Physical Properties

Property code	Value	Unit	Source
gf	-926.75	kJ/mol	Joback Method
hf	-1147.28	kJ/mol	Joback Method
hfus	32.20	kJ/mol	Joback Method
hvap	74.99	kJ/mol	Joback Method
log10ws	-0.03		Crippen Method
logp	-1.134		Crippen Method
mcvol	131.250	ml/mol	McGowan Method
pc	3891.64	kPa	Joback Method
tb	685.39	K	Joback Method
tc	865.43	K	Joback Method
tf	477.50	K	Joback Method
vc	0.521	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	359.70	J/mol×K	685.39	Joback Method
cpg	366.55	J/mol×K	715.40	Joback Method
cpg	372.92	J/mol×K	745.40	Joback Method
cpg	378.84	J/mol×K	775.41	Joback Method
cpg	384.32	J/mol×K	805.41	Joback Method
cpg	389.39	J/mol×K	835.42	Joback Method
cpg	394.08	J/mol×K	865.43	Joback Method
hsubt	67.00	kJ/mol	348.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C400588&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