Glycine, N-pentafluoropropionyl-, methyl ester

Inchi: InChI=1S/C6H6F5NO3/c1-15-3(13)2-12-4(14)5(7,8)6(9,10)11/h2H2,1H3,(H,12,14)
InchiKey: VQVKUEWRCJYNCA-UHFFFAOYSA-N
Formula: C6H6F5NO3
SMILES: COC(=O)CNC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 235.11

Physical Properties

Property code	Value	Unit	Source
gf	-1242.18	kJ/mol	Joback Method
hf	-1469.13	kJ/mol	Joback Method
hfus	21.35	kJ/mol	Joback Method
hvap	44.61	kJ/mol	Joback Method
log10ws	-1.14		Crippen Method
logp	0.473		Crippen Method
mcvol	123.240	ml/mol	McGowan Method
pc	2893.62	kPa	Joback Method
rinpol	971.00		NIST Webbook
rinpol	971.00		NIST Webbook
tb	506.90	K	Joback Method
tc	675.79	K	Joback Method
tf	339.92	K	Joback Method
vc	0.504	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	305.09	J/mol×K	506.90	Joback Method
cpg	314.24	J/mol×K	535.05	Joback Method
cpg	322.81	J/mol×K	563.20	Joback Method
cpg	330.85	J/mol×K	591.34	Joback Method
cpg	338.37	J/mol×K	619.49	Joback Method
cpg	345.39	J/mol×K	647.64	Joback Method
cpg	351.94	J/mol×K	675.79	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374295&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
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