Glycine, N-heptafluorobutyryl-, methyl ester

Inchi: InChI=1S/C7H6F7NO3/c1-18-3(16)2-15-4(17)5(8,9)6(10,11)7(12,13)14/h2H2,1H3,(H,15,
InchiKey: IPSZMIRIAURPSU-UHFFFAOYSA-N
Formula: C7H6F7NO3
SMILES: COC(=O)CNC(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 285.12

Physical Properties

Property code	Value	Unit	Source
gf	-1620.54	kJ/mol	Joback Method
hf	-1890.74	kJ/mol	Joback Method
hfus	22.69	kJ/mol	Joback Method
hvap	43.91	kJ/mol	Joback Method
log10ws	-1.87		Crippen Method
logp	1.109		Crippen Method
mcvol	140.870	ml/mol	McGowan Method
pc	2436.25	kPa	Joback Method
rinpol	1013.00		NIST Webbook
tb	525.09	K	Joback Method
tc	687.13	K	Joback Method
tf	354.79	K	Joback Method
vc	0.586	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	368.54	J/mol×K	525.09	Joback Method
cpg	378.27	J/mol×K	552.10	Joback Method
cpg	387.35	J/mol×K	579.10	Joback Method
cpg	395.80	J/mol×K	606.11	Joback Method
cpg	403.65	J/mol×K	633.11	Joback Method
cpg	410.95	J/mol×K	660.12	Joback Method
cpg	417.72	J/mol×K	687.13	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374296&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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