Glycine, N-chlorodifluoroacetyl-, ethyl ester

Inchi: InChI=1S/C6H8ClF2NO3/c1-2-13-4(11)3-10-5(12)6(7,8)9/h2-3H2,1H3,(H,10,12)
InchiKey: YMTCSJDPNOTFEL-UHFFFAOYSA-N
Formula: C6H8ClF2NO3
SMILES: CCOC(=O)CNC(=O)C(F)(F)Cl
Mol. weight [g/mol]: 215.58

Physical Properties

Property code	Value	Unit	Source
gf	-672.52	kJ/mol	Joback Method
hf	-887.79	kJ/mol	Joback Method
hfus	23.72	kJ/mol	Joback Method
hvap	52.74	kJ/mol	Joback Method
log10ws	-1.12		Crippen Method
logp	0.497		Crippen Method
mcvol	130.170	ml/mol	McGowan Method
pc	3156.17	kPa	Joback Method
rinpol	1184.00		NIST Webbook
tb	549.75	K	Joback Method
tc	738.42	K	Joback Method
tf	365.65	K	Joback Method
vc	0.510	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	300.38	J/mol×K	549.75	Joback Method
cpg	309.48	J/mol×K	581.19	Joback Method
cpg	318.05	J/mol×K	612.64	Joback Method
cpg	326.10	J/mol×K	644.08	Joback Method
cpg	333.64	J/mol×K	675.53	Joback Method
cpg	340.70	J/mol×K	706.97	Joback Method
cpg	347.29	J/mol×K	738.42	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375628&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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