p-Fluoro-L-phenylalanine, N-chlorodifluoroacetyl-, ethyl ester

Inchi: InChI=1S/C13H13ClF3NO3/c1-2-21-11(19)10(18-12(20)13(14,16)17)7-8-3-5-9(15)6-4-8/h
InchiKey: MHBNBWPSGRXSLW-UHFFFAOYSA-N
Formula: C13H13ClF3NO3
SMILES: CCOC(=O)C(Cc1ccc(F)cc1)NC(=O)C(F)(F)Cl
Mol. weight [g/mol]: 323.69

Physical Properties

Property code	Value	Unit	Source
gf	-708.05	kJ/mol	Joback Method
hf	-1008.60	kJ/mol	Joback Method
hfus	35.06	kJ/mol	Joback Method
hvap	70.06	kJ/mol	Joback Method
log10ws	-3.60		Crippen Method
logp	2.248		Crippen Method
mcvol	206.810	ml/mol	McGowan Method
pc	2117.78	kPa	Joback Method
rinpol	1245.00		NIST Webbook
rinpol	1245.00		NIST Webbook
tb	740.40	K	Joback Method
tc	943.90	K	Joback Method
tf	469.07	K	Joback Method
vc	0.806	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	565.41	J/mol×K	740.40	Joback Method
cpg	576.91	J/mol×K	774.32	Joback Method
cpg	587.54	J/mol×K	808.23	Joback Method
cpg	597.35	J/mol×K	842.15	Joback Method
cpg	606.37	J/mol×K	876.07	Joback Method
cpg	614.65	J/mol×K	909.98	Joback Method
cpg	622.24	J/mol×K	943.90	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375826&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