DL-Phenylalanine, N-chlorodifluoroacetyl-, ethyl ester

Inchi: InChI=1S/C13H14ClF2NO3/c1-2-20-11(18)10(17-12(19)13(14,15)16)8-9-6-4-3-5-7-9/h3-
InchiKey: GBLBQWFRENCJNP-UHFFFAOYSA-N
Formula: C13H14ClF2NO3
SMILES: CCOC(=O)C(Cc1ccccc1)NC(=O)C(F)(F)Cl
Mol. weight [g/mol]: 305.70

Physical Properties

Property code	Value	Unit	Source
gf	-503.61	kJ/mol	Joback Method
hf	-801.02	kJ/mol	Joback Method
hfus	32.37	kJ/mol	Joback Method
hvap	70.21	kJ/mol	Joback Method
log10ws	-3.27		Crippen Method
logp	2.109		Crippen Method
mcvol	205.040	ml/mol	McGowan Method
pc	2239.76	kPa	Joback Method
rinpol	1249.00		NIST Webbook
rinpol	1249.00		NIST Webbook
tb	736.15	K	Joback Method
tc	946.31	K	Joback Method
tf	455.96	K	Joback Method
vc	0.788	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	558.88	J/mol×K	736.15	Joback Method
cpg	571.01	J/mol×K	771.18	Joback Method
cpg	582.19	J/mol×K	806.20	Joback Method
cpg	592.48	J/mol×K	841.23	Joback Method
cpg	601.93	J/mol×K	876.25	Joback Method
cpg	610.59	J/mol×K	911.28	Joback Method
cpg	618.51	J/mol×K	946.31	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375698&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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