phenylalanine, trifluoroacetyl-isopropyl ester

Inchi: InChI=1S/C14H16F3NO3/c1-9(2)21-12(19)11(18-13(20)14(15,16)17)8-10-6-4-3-5-7-10/h
InchiKey: YULLKCJHWWNQEE-UHFFFAOYSA-N
Formula: C14H16F3NO3
SMILES: CC(C)OC(=O)C(Cc1ccccc1)NC(=O)C(F)(F)F
Mol. weight [g/mol]: 303.28

Physical Properties

Property code	Value	Unit	Source
gf	-680.51	kJ/mol	Joback Method
hf	-1007.31	kJ/mol	Joback Method
hfus	30.32	kJ/mol	Joback Method
hvap	66.85	kJ/mol	Joback Method
log10ws	-3.50		Crippen Method
logp	2.228		Crippen Method
mcvol	208.660	ml/mol	McGowan Method
pc	2049.31	kPa	Joback Method
rinpol	1571.00		NIST Webbook
rinpol	1571.00		NIST Webbook
tb	720.43	K	Joback Method
tc	920.58	K	Joback Method
tf	422.90	K	Joback Method
vc	0.807	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	595.21	J/mol×K	720.43	Joback Method
cpg	608.53	J/mol×K	753.79	Joback Method
cpg	620.90	J/mol×K	787.15	Joback Method
cpg	632.35	J/mol×K	820.51	Joback Method
cpg	642.93	J/mol×K	853.86	Joback Method
cpg	652.70	J/mol×K	887.22	Joback Method
cpg	661.70	J/mol×K	920.58	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=R267962&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