l-Phenylalanine, n-pentafluoropropionyl-, isohexyl ester

Inchi: InChI=1S/C18H22F5NO3/c1-12(2)7-6-10-27-15(25)14(11-13-8-4-3-5-9-13)24-16(26)17(1

InchiKey: JQUMOOLSHNOQGO-UHFFFAOYSA-N

Formula: C18H22F5NO3

SMILES: CC(C)CCCOC(=O)C(Cc1ccccc1)NC(=O)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 395.36

Physical Properties

Property code	Value	Unit	Source
gf	-1033.61	kJ/mol	Joback Method
hf	-1490.84	kJ/mol	Joback Method
hfus	39.43	kJ/mol	Joback Method
hvap	72.82	kJ/mol	Joback Method
log10ws	-5.13		Crippen Method
logp	3.891		Crippen Method
mcvol	268.560	ml/mol	McGowan Method
pc	1409.07	kPa	Joback Method
rinpol	1839.00		NIST Webbook
tb	807.26	K	Joback Method
tc	1000.41	K	Joback Method
tf	471.58	K	Joback Method
vc	1.056	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	832.97	J/mol×K	807.26	Joback Method
cpg	846.74	J/mol×K	839.45	Joback Method
cpg	859.54	J/mol×K	871.64	Joback Method
cpg	871.44	J/mol×K	903.84	Joback Method
cpg	882.49	J/mol×K	936.03	Joback Method
cpg	892.78	J/mol×K	968.22	Joback Method
cpg	902.35	J/mol×K	1000.41	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=U321021&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