l-Phenylalanine, n-pentafluoropropionyl-, propyl ester

Inchi: InChI=1S/C15H16F5NO3/c1-2-8-24-12(22)11(9-10-6-4-3-5-7-10)21-13(23)14(16,17)15(1

InchiKey: ZBHDETAIWKHOPT-UHFFFAOYSA-N

Formula: C15H16F5NO3

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

Mol. weight [g/mol]: 353.28

Physical Properties

Property code	Value	Unit	Source
gf	-1056.43	kJ/mol	Joback Method
hf	-1423.64	kJ/mol	Joback Method
hfus	35.18	kJ/mol	Joback Method
hvap	66.53	kJ/mol	Joback Method
log10ws	-4.12		Crippen Method
logp	2.865		Crippen Method
mcvol	226.290	ml/mol	McGowan Method
pc	1759.49	kPa	Joback Method
rinpol	1622.00		NIST Webbook
rinpol	1622.00		NIST Webbook
tb	739.06	K	Joback Method
tc	930.03	K	Joback Method
tf	452.77	K	Joback Method
vc	0.894	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	666.33	J/mol×K	739.06	Joback Method
cpg	679.05	J/mol×K	770.89	Joback Method
cpg	690.84	J/mol×K	802.72	Joback Method
cpg	701.76	J/mol×K	834.54	Joback Method
cpg	711.88	J/mol×K	866.37	Joback Method
cpg	721.26	J/mol×K	898.20	Joback Method
cpg	729.95	J/mol×K	930.03	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321018&Units=SI

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