l-Phenylalanine, n-pentafluoropropionyl-, pentadecyl ester

Inchi: InChI=1S/C27H40F5NO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-17-20-36-24(34)23(21-22-18-1

InchiKey: SKIHBNORUZAWOW-UHFFFAOYSA-N

Formula: C27H40F5NO3

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

Mol. weight [g/mol]: 521.60

Physical Properties

Property code	Value	Unit	Source
gf	-955.39	kJ/mol	Joback Method
hf	-1671.32	kJ/mol	Joback Method
hfus	66.26	kJ/mol	Joback Method
hvap	93.25	kJ/mol	Joback Method
log10ws	-9.14		Crippen Method
logp	7.546		Crippen Method
mcvol	395.370	ml/mol	McGowan Method
pc	799.79	kPa	Joback Method
rinpol	2780.00		NIST Webbook
tb	1013.62	K	Joback Method
tc	1250.27	K	Joback Method
tf	588.01	K	Joback Method
vc	1.567	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1372.56	J/mol×K	1013.62	Joback Method
cpg	1390.57	J/mol×K	1053.06	Joback Method
cpg	1407.34	J/mol×K	1092.50	Joback Method
cpg	1423.03	J/mol×K	1131.94	Joback Method
cpg	1437.79	J/mol×K	1171.39	Joback Method
cpg	1451.80	J/mol×K	1210.83	Joback Method
cpg	1465.22	J/mol×K	1250.27	Joback Method

Sources

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=U321029&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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