l-Phenylalanine, n-pentafluoropropionyl-, undecyl ester

Inchi: InChI=1S/C23H32F5NO3/c1-2-3-4-5-6-7-8-9-13-16-32-20(30)19(17-18-14-11-10-12-15-1

InchiKey: OAKAJNFXZMKPEU-UHFFFAOYSA-N

Formula: C23H32F5NO3

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

Mol. weight [g/mol]: 465.50

Physical Properties

Property code	Value	Unit	Source
gf	-989.07	kJ/mol	Joback Method
hf	-1588.76	kJ/mol	Joback Method
hfus	55.90	kJ/mol	Joback Method
hvap	84.34	kJ/mol	Joback Method
log10ws	-7.47		Crippen Method
logp	5.986		Crippen Method
mcvol	339.010	ml/mol	McGowan Method
pc	1006.53	kPa	Joback Method
rinpol	2379.00		NIST Webbook
tb	922.10	K	Joback Method
tc	1128.92	K	Joback Method
tf	542.93	K	Joback Method
vc	1.343	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1125.97	J/mol×K	922.10	Joback Method
cpg	1141.54	J/mol×K	956.57	Joback Method
cpg	1156.04	J/mol×K	991.04	Joback Method
cpg	1169.58	J/mol×K	1025.51	Joback Method
cpg	1182.24	J/mol×K	1059.98	Joback Method
cpg	1194.13	J/mol×K	1094.45	Joback Method
cpg	1205.34	J/mol×K	1128.92	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=U321026&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