l-Phenylalanine, n-heptafluorobutyryl-, undecyl ester

Inchi: InChI=1S/C24H32F7NO3/c1-2-3-4-5-6-7-8-9-13-16-35-20(33)19(17-18-14-11-10-12-15-1

InchiKey: DEVCZRFCLVHFTP-UHFFFAOYSA-N

Formula: C24H32F7NO3

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

Mol. weight [g/mol]: 515.50

Physical Properties

Property code	Value	Unit	Source
gf	-1367.43	kJ/mol	Joback Method
hf	-2010.37	kJ/mol	Joback Method
hfus	57.24	kJ/mol	Joback Method
hvap	83.64	kJ/mol	Joback Method
log10ws	-8.20		Crippen Method
logp	6.621		Crippen Method
mcvol	356.640	ml/mol	McGowan Method
pc	907.79	kPa	Joback Method
rinpol	2391.00		NIST Webbook
tb	940.29	K	Joback Method
tc	1152.56	K	Joback Method
tf	557.80	K	Joback Method
vc	1.423	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1200.92	J/mol×K	940.29	Joback Method
cpg	1216.64	J/mol×K	975.67	Joback Method
cpg	1231.34	J/mol×K	1011.05	Joback Method
cpg	1245.15	J/mol×K	1046.43	Joback Method
cpg	1258.21	J/mol×K	1081.80	Joback Method
cpg	1270.64	J/mol×K	1117.18	Joback Method
cpg	1282.57	J/mol×K	1152.56	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=U321115&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