l-Phenylalanine, n-heptafluorobutyryl-, hexadecyl ester

Inchi: InChI=1S/C29H42F7NO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-18-21-40-25(38)24(22-23-1

InchiKey: GPYLMDHCDSFFLE-UHFFFAOYSA-N

Formula: C29H42F7NO3

SMILES: CCCCCCCCCCCCCCCCOC(=O)C(Cc1ccccc1)N=C(O)C(F)(F)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 585.64

Physical Properties

Property code	Value	Unit	Source
hf	-2134.26	kJ/mol	Joback Method
hvap	101.66	kJ/mol	Joback Method
log10ws	-10.31		Crippen Method
logp	9.412		Crippen Method
mcvol	427.090	ml/mol	McGowan Method
pc	663.23	kPa	Joback Method
rinpol	2915.00		NIST Webbook
rinpol	2915.00		NIST Webbook
tb	1119.39	K	Joback Method
tc	1420.47	K	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=U321119&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

hf: Enthalpy of formation 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