l-Phenylalanine, n-pentafluoropropionyl-, octadecyl ester

Inchi: InChI=1S/C30H46F5NO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-20-23-39-27(37)26(2

InchiKey: UJNQVBXSVXIMAN-UHFFFAOYSA-N

Formula: C30H46F5NO3

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

Mol. weight [g/mol]: 563.68

Physical Properties

Property code	Value	Unit	Source
gf	-930.13	kJ/mol	Joback Method
hf	-1733.24	kJ/mol	Joback Method
hfus	74.03	kJ/mol	Joback Method
hvap	99.92	kJ/mol	Joback Method
log10ws	-10.40		Crippen Method
logp	8.716		Crippen Method
mcvol	437.640	ml/mol	McGowan Method
pc	683.86	kPa	Joback Method
rinpol	3235.00		NIST Webbook
tb	1082.26	K	Joback Method
tc	1355.09	K	Joback Method
tf	621.82	K	Joback Method
vc	1.734	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1562.91	J/mol×K	1082.26	Joback Method
cpg	1583.72	J/mol×K	1127.73	Joback Method
cpg	1603.11	J/mol×K	1173.20	Joback Method
cpg	1621.34	J/mol×K	1218.68	Joback Method
cpg	1638.70	J/mol×K	1264.15	Joback Method
cpg	1655.45	J/mol×K	1309.62	Joback Method
cpg	1671.86	J/mol×K	1355.09	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=U321032&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