l-Phenylalanine, n-heptafluorobutyryl-, octadecyl ester

Inchi: InChI=1S/C31H46F7NO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-20-23-42-27(40)26(2

InchiKey: TXNIOWFWTPLLHT-UHFFFAOYSA-N

Formula: C31H46F7NO3

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

Mol. weight [g/mol]: 613.69

Physical Properties

Property code	Value	Unit	Source
gf	-1308.49	kJ/mol	Joback Method
hf	-2154.85	kJ/mol	Joback Method
hfus	75.37	kJ/mol	Joback Method
hvap	99.22	kJ/mol	Joback Method
log10ws	-11.13		Crippen Method
logp	9.352		Crippen Method
mcvol	455.270	ml/mol	McGowan Method
pc	627.82	kPa	Joback Method
rinpol	3241.00		NIST Webbook
rinpol	3241.00		NIST Webbook
tb	1100.45	K	Joback Method
tc	1392.90	K	Joback Method
tf	636.69	K	Joback Method
vc	1.815	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1640.13	J/mol×K	1100.45	Joback Method
cpg	1662.83	J/mol×K	1149.19	Joback Method
cpg	1684.36	J/mol×K	1197.93	Joback Method
cpg	1705.14	J/mol×K	1246.68	Joback Method
cpg	1725.55	J/mol×K	1295.42	Joback Method
cpg	1746.00	J/mol×K	1344.16	Joback Method
cpg	1766.89	J/mol×K	1392.90	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321121&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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

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