l-Phenylalanine, n-pentafluoropropionyl-, hexadecyl ester

Inchi: InChI=1S/C28H42F5NO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-18-21-37-25(35)24(22-23-1
InchiKey: GHALAEIBDPQHRB-UHFFFAOYSA-N
Formula: C28H42F5NO3
SMILES: CCCCCCCCCCCCCCCCOC(=O)C(Cc1ccccc1)NC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 535.63

Physical Properties

Property code	Value	Unit	Source
gf	-946.97	kJ/mol	Joback Method
hf	-1691.96	kJ/mol	Joback Method
hfus	68.85	kJ/mol	Joback Method
hvap	95.47	kJ/mol	Joback Method
log10ws	-9.56		Crippen Method
logp	7.936		Crippen Method
mcvol	409.460	ml/mol	McGowan Method
pc	758.07	kPa	Joback Method
rinpol	2908.00		NIST Webbook
tb	1036.50	K	Joback Method
tc	1283.72	K	Joback Method
tf	599.28	K	Joback Method
vc	1.623	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1435.53	J/mol×K	1036.50	Joback Method
cpg	1454.37	J/mol×K	1077.70	Joback Method
cpg	1471.90	J/mol×K	1118.91	Joback Method
cpg	1488.32	J/mol×K	1160.11	Joback Method
cpg	1503.82	J/mol×K	1201.32	Joback Method
cpg	1518.59	J/mol×K	1242.52	Joback Method
cpg	1532.83	J/mol×K	1283.72	Joback Method

Sources

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=U321030&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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