l-Phenylalanine, n-pentafluoropropionyl-, tetradecyl ester

Inchi: InChI=1S/C26H38F5NO3/c1-2-3-4-5-6-7-8-9-10-11-12-16-19-35-23(33)22(20-21-17-14-1

InchiKey: OGTHSGNFIQCTDZ-UHFFFAOYSA-N

Formula: C26H38F5NO3

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

Mol. weight [g/mol]: 507.58

Physical Properties

Property code	Value	Unit	Source
gf	-963.81	kJ/mol	Joback Method
hf	-1650.68	kJ/mol	Joback Method
hfus	63.67	kJ/mol	Joback Method
hvap	91.02	kJ/mol	Joback Method
log10ws	-8.72		Crippen Method
logp	7.156		Crippen Method
mcvol	381.280	ml/mol	McGowan Method
pc	845.05	kPa	Joback Method
rinpol	2669.00		NIST Webbook
tb	990.74	K	Joback Method
tc	1218.15	K	Joback Method
tf	576.74	K	Joback Method
vc	1.510	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1310.08	J/mol×K	990.74	Joback Method
cpg	1327.37	J/mol×K	1028.64	Joback Method
cpg	1343.47	J/mol×K	1066.54	Joback Method
cpg	1358.51	J/mol×K	1104.45	Joback Method
cpg	1372.64	J/mol×K	1142.35	Joback Method
cpg	1386.00	J/mol×K	1180.25	Joback Method
cpg	1398.73	J/mol×K	1218.15	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=U321028&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