l-Phenylalanine, n-pentafluoropropionyl-, decyl ester

Inchi: InChI=1S/C22H30F5NO3/c1-2-3-4-5-6-7-8-12-15-31-19(29)18(16-17-13-10-9-11-14-17)2

InchiKey: UVEMRDVEVRJYRW-UHFFFAOYSA-N

Formula: C22H30F5NO3

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

Mol. weight [g/mol]: 451.47

Physical Properties

Property code	Value	Unit	Source
gf	-997.49	kJ/mol	Joback Method
hf	-1568.12	kJ/mol	Joback Method
hfus	53.31	kJ/mol	Joback Method
hvap	82.11	kJ/mol	Joback Method
log10ws	-7.05		Crippen Method
logp	5.595		Crippen Method
mcvol	324.920	ml/mol	McGowan Method
pc	1070.76	kPa	Joback Method
rinpol	2277.00		NIST Webbook
rinpol	2277.00		NIST Webbook
tb	899.22	K	Joback Method
tc	1101.26	K	Joback Method
tf	531.66	K	Joback Method
vc	1.286	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1065.82	J/mol×K	899.22	Joback Method
cpg	1080.94	J/mol×K	932.89	Joback Method
cpg	1095.02	J/mol×K	966.57	Joback Method
cpg	1108.15	J/mol×K	1000.24	Joback Method
cpg	1120.43	J/mol×K	1033.92	Joback Method
cpg	1131.94	J/mol×K	1067.59	Joback Method
cpg	1142.77	J/mol×K	1101.26	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321025&Units=SI

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