l-Phenylalanine, n-pentafluoropropionyl-, nonyl ester

Inchi: InChI=1S/C21H28F5NO3/c1-2-3-4-5-6-7-11-14-30-18(28)17(15-16-12-9-8-10-13-16)27-1

InchiKey: SJYNVAKMXGSJME-UHFFFAOYSA-N

Formula: C21H28F5NO3

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

Mol. weight [g/mol]: 437.44

Physical Properties

Property code	Value	Unit	Source
gf	-1005.91	kJ/mol	Joback Method
hf	-1547.48	kJ/mol	Joback Method
hfus	50.72	kJ/mol	Joback Method
hvap	79.89	kJ/mol	Joback Method
log10ws	-6.63		Crippen Method
logp	5.205		Crippen Method
mcvol	310.830	ml/mol	McGowan Method
pc	1141.34	kPa	Joback Method
rinpol	2178.00		NIST Webbook
rinpol	2178.00		NIST Webbook
tb	876.34	K	Joback Method
tc	1074.53	K	Joback Method
tf	520.39	K	Joback Method
vc	1.230	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1006.35	J/mol×K	876.34	Joback Method
cpg	1021.05	J/mol×K	909.37	Joback Method
cpg	1034.75	J/mol×K	942.40	Joback Method
cpg	1047.52	J/mol×K	975.44	Joback Method
cpg	1059.45	J/mol×K	1008.47	Joback Method
cpg	1070.62	J/mol×K	1041.50	Joback Method
cpg	1081.10	J/mol×K	1074.53	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=U321024&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