l-Phenylalanine, n-pentafluoropropionyl-, heptyl ester

Inchi: InChI=1S/C19H24F5NO3/c1-2-3-4-5-9-12-28-16(26)15(13-14-10-7-6-8-11-14)25-17(27)1

InchiKey: BUCMQTRROBFHOK-UHFFFAOYSA-N

Formula: C19H24F5NO3

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

Mol. weight [g/mol]: 409.39

Physical Properties

Property code	Value	Unit	Source
gf	-1022.75	kJ/mol	Joback Method
hf	-1506.20	kJ/mol	Joback Method
hfus	45.54	kJ/mol	Joback Method
hvap	75.44	kJ/mol	Joback Method
log10ws	-5.79		Crippen Method
logp	4.425		Crippen Method
mcvol	282.650	ml/mol	McGowan Method
pc	1305.17	kPa	Joback Method
rinpol	1990.00		NIST Webbook
rinpol	1990.00		NIST Webbook
tb	830.58	K	Joback Method
tc	1023.58	K	Joback Method
tf	497.85	K	Joback Method
vc	1.119	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	889.59	J/mol×K	830.58	Joback Method
cpg	903.58	J/mol×K	862.75	Joback Method
cpg	916.60	J/mol×K	894.91	Joback Method
cpg	928.73	J/mol×K	927.08	Joback Method
cpg	940.04	J/mol×K	959.25	Joback Method
cpg	950.59	J/mol×K	991.41	Joback Method
cpg	960.45	J/mol×K	1023.58	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321022&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

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