l-Phenylalanine, n-heptafluorobutyryl-, isohexyl ester

Inchi: InChI=1S/C19H22F7NO3/c1-12(2)7-6-10-30-15(28)14(11-13-8-4-3-5-9-13)27-16(29)17(2

InchiKey: UMLTWDDGQUGIAN-UHFFFAOYSA-N

Formula: C19H22F7NO3

SMILES: CC(C)CCCOC(=O)C(Cc1ccccc1)NC(=O)C(F)(F)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 445.37

Physical Properties

Property code	Value	Unit	Source
gf	-1411.97	kJ/mol	Joback Method
hf	-1912.45	kJ/mol	Joback Method
hfus	40.76	kJ/mol	Joback Method
hvap	72.12	kJ/mol	Joback Method
log10ws	-5.87		Crippen Method
logp	4.526		Crippen Method
mcvol	286.190	ml/mol	McGowan Method
pc	1247.73	kPa	Joback Method
rinpol	1860.00		NIST Webbook
rinpol	1860.00		NIST Webbook
tb	825.45	K	Joback Method
tc	1016.77	K	Joback Method
tf	486.45	K	Joback Method
vc	1.137	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	906.37	J/mol×K	825.45	Joback Method
cpg	919.80	J/mol×K	857.34	Joback Method
cpg	932.27	J/mol×K	889.22	Joback Method
cpg	943.89	J/mol×K	921.11	Joback Method
cpg	954.72	J/mol×K	953.00	Joback Method
cpg	964.85	J/mol×K	984.88	Joback Method
cpg	974.37	J/mol×K	1016.77	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=U321111&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