l-Phenylalanine, n-heptafluorobutyryl-, butyl ester

Inchi: InChI=1S/C17H18F7NO3/c1-2-3-9-28-13(26)12(10-11-7-5-4-6-8-11)25-14(27)15(18,19)1

InchiKey: OCQYHUKFEDQUNZ-UHFFFAOYSA-N

Formula: C17H18F7NO3

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

Mol. weight [g/mol]: 417.32

Physical Properties

Property code	Value	Unit	Source
gf	-1426.37	kJ/mol	Joback Method
hf	-1865.89	kJ/mol	Joback Method
hfus	39.11	kJ/mol	Joback Method
hvap	68.05	kJ/mol	Joback Method
log10ws	-5.27		Crippen Method
logp	3.890		Crippen Method
mcvol	258.010	ml/mol	McGowan Method
pc	1427.22	kPa	Joback Method
rinpol	1732.00		NIST Webbook
tb	780.13	K	Joback Method
tc	967.18	K	Joback Method
tf	478.91	K	Joback Method
vc	1.032	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	793.25	J/mol×K	780.13	Joback Method
cpg	805.92	J/mol×K	811.30	Joback Method
cpg	817.67	J/mol×K	842.48	Joback Method
cpg	828.58	J/mol×K	873.65	Joback Method
cpg	838.72	J/mol×K	904.83	Joback Method
cpg	848.17	J/mol×K	936.00	Joback Method
cpg	857.00	J/mol×K	967.18	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=U321109&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