l-Phenylalanine, n-pentafluoropropionyl-, isobutyl ester

Inchi: InChI=1S/C16H18F5NO3/c1-10(2)9-25-13(23)12(8-11-6-4-3-5-7-11)22-14(24)15(17,18)1

InchiKey: OBUMSQYNXSUXLR-UHFFFAOYSA-N

Formula: C16H18F5NO3

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

Mol. weight [g/mol]: 367.31

Physical Properties

Property code	Value	Unit	Source
gf	-1050.45	kJ/mol	Joback Method
hf	-1449.56	kJ/mol	Joback Method
hfus	34.25	kJ/mol	Joback Method
hvap	68.37	kJ/mol	Joback Method
log10ws	-4.30		Crippen Method
logp	3.111		Crippen Method
mcvol	240.380	ml/mol	McGowan Method
pc	1636.45	kPa	Joback Method
rinpol	1666.00		NIST Webbook
rinpol	1666.00		NIST Webbook
tb	761.50	K	Joback Method
tc	954.28	K	Joback Method
tf	449.04	K	Joback Method
vc	0.945	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	721.29	J/mol×K	761.50	Joback Method
cpg	734.48	J/mol×K	793.63	Joback Method
cpg	746.72	J/mol×K	825.76	Joback Method
cpg	758.06	J/mol×K	857.89	Joback Method
cpg	768.56	J/mol×K	890.02	Joback Method
cpg	778.29	J/mol×K	922.15	Joback Method
cpg	787.31	J/mol×K	954.28	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=U321019&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