l-Phenylalanine, n-pentafluoropropionyl-, dodecyl ester

Inchi: InChI=1S/C24H34F5NO3/c1-2-3-4-5-6-7-8-9-10-14-17-33-21(31)20(18-19-15-12-11-13-1

InchiKey: NJMPKMAKZGSKSM-UHFFFAOYSA-N

Formula: C24H34F5NO3

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

Mol. weight [g/mol]: 479.52

Physical Properties

Property code	Value	Unit	Source
gf	-980.65	kJ/mol	Joback Method
hf	-1609.40	kJ/mol	Joback Method
hfus	58.49	kJ/mol	Joback Method
hvap	86.57	kJ/mol	Joback Method
log10ws	-7.89		Crippen Method
logp	6.376		Crippen Method
mcvol	353.100	ml/mol	McGowan Method
pc	947.91	kPa	Joback Method
rinpol	2475.00		NIST Webbook
tb	944.98	K	Joback Method
tc	1157.56	K	Joback Method
tf	554.20	K	Joback Method
vc	1.399	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1186.76	J/mol×K	944.98	Joback Method
cpg	1202.83	J/mol×K	980.41	Joback Method
cpg	1217.81	J/mol×K	1015.84	Joback Method
cpg	1231.78	J/mol×K	1051.27	Joback Method
cpg	1244.88	J/mol×K	1086.70	Joback Method
cpg	1257.19	J/mol×K	1122.13	Joback Method
cpg	1268.84	J/mol×K	1157.56	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=U321027&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