l-Phenylalanine, n-pentafluoropropionyl-, ethyl ester

Inchi: InChI=1S/C14H14F5NO3/c1-2-23-11(21)10(8-9-6-4-3-5-7-9)20-12(22)13(15,16)14(17,18

InchiKey: SWIIZDOASUPMEX-UHFFFAOYSA-N

Formula: C14H14F5NO3

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

Mol. weight [g/mol]: 339.26

Physical Properties

Property code	Value	Unit	Source
gf	-1064.85	kJ/mol	Joback Method
hf	-1403.00	kJ/mol	Joback Method
hfus	32.59	kJ/mol	Joback Method
hvap	64.31	kJ/mol	Joback Method
log10ws	-3.70		Crippen Method
logp	2.475		Crippen Method
mcvol	212.200	ml/mol	McGowan Method
pc	1910.24	kPa	Joback Method
rinpol	1541.00		NIST Webbook
tb	716.18	K	Joback Method
tc	908.07	K	Joback Method
tf	441.50	K	Joback Method
vc	0.839	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	613.00	J/mol×K	716.18	Joback Method
cpg	625.37	J/mol×K	748.16	Joback Method
cpg	636.82	J/mol×K	780.14	Joback Method
cpg	647.42	J/mol×K	812.13	Joback Method
cpg	657.21	J/mol×K	844.11	Joback Method
cpg	666.26	J/mol×K	876.09	Joback Method
cpg	674.62	J/mol×K	908.07	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=U321017&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