

L-Phenylalanine, N-(4-fluorobenzoyl)-, methyl ester

Inchi:	InChI=1S/C17H16FNO3/c1-22-17(21)15(11-12-5-3-2-4-6-12)19-16(20)13-7-9-14(18)10-8
InchiKey:	NUEPYHOVUXEGDD-UHFFFAOYSA-N
Formula:	C17H16FNO3
SMILES:	COC(=O)C(Cc1ccccc1)NC(=O)c1ccc(F)cc1
Mol. weight [g/mol]:	301.31

Physical Properties

Property code	Value	Unit	Source
gf	-163.25	kJ/mol	Joback Method
hf	-437.92	kJ/mol	Joback Method
hfus	36.52	kJ/mol	Joback Method
hvap	79.78	kJ/mol	Joback Method
log10ws	-3.99		Crippen Method
logp	2.340		Crippen Method
mvol	223.630	ml/mol	McGowan Method
pc	2229.20	kPa	Joback Method
rinpol	2196.00		NIST Webbook
rinpol	2196.00		NIST Webbook
tb	825.86	K	Joback Method
tc	1054.31	K	Joback Method
tf	507.05	K	Joback Method
vc	0.849	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	647.33	J/molxK	825.86	Joback Method
cpg	660.26	J/molxK	863.94	Joback Method
cpg	672.02	J/molxK	902.01	Joback Method
cpg	682.68	J/molxK	940.09	Joback Method
cpg	692.27	J/molxK	978.16	Joback Method
cpg	700.86	J/molxK	1016.24	Joback Method
cpg	708.50	J/molxK	1054.31	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=U299608&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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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