L-Phenylalanine, N-(3-fluorobenzoyl)-, methyl ester

Inchi: InChI=1S/C17H16FNO3/c1-22-17(21)15(10-12-6-3-2-4-7-12)19-16(20)13-8-5-9-14(18)11

InchiKey: SQUNXHNZPDBHRA-UHFFFAOYSA-N

Formula: C17H16FNO3

SMILES: COC(=O)C(Cc1ccccc1)NC(=O)c1cccc(F)c1

Mol. weight [g/mol]: 301.32

Physical Properties

Property code	Value	Unit	Source
hfus	36.52	kJ/mol	Joback Method
ie	8.77	eV	Cheméo Relay (1.0)
log10ws	-3.86		Cheméo Relay (1.0)
logp	2.340		Crippen Method
mcvol	223.630	ml/mol	McGowan Method
rinpol	2190.00		NIST Webbook
rinpol	2190.00		NIST Webbook
tf	348.99	K	Cheméo Relay (1.0)

Temperature Dependent Properties

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

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299679&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point