L-Phenylalanine, N-(2,6-difluorobenzoyl)-, methyl ester

Inchi: InChI=1S/C17H15F2NO3/c1-23-17(22)14(10-11-6-3-2-4-7-11)20-16(21)15-12(18)8-5-9-1

InchiKey: JAKBXLAQIOZZHD-UHFFFAOYSA-N

Formula: C17H15F2NO3

SMILES: COC(=O)C(Cc1ccccc1)NC(=O)c1c(F)cccc1F

Mol. weight [g/mol]: 319.31

Physical Properties

Property code	Value	Unit	Source
hfus	39.21	kJ/mol	Joback Method
log10ws	-4.32		Cheméo Relay (1.0)
logp	2.479		Crippen Method
mcvol	225.400	ml/mol	McGowan Method
rinpol	2216.00		NIST Webbook
rinpol	2216.00		NIST Webbook
tb	625.57	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	653.48	J/mol×K	830.11	Joback Method
cpg	665.78	J/mol×K	867.04	Joback Method
cpg	676.99	J/mol×K	903.97	Joback Method
cpg	687.16	J/mol×K	940.90	Joback Method
cpg	696.32	J/mol×K	977.82	Joback Method
cpg	704.51	J/mol×K	1014.75	Joback Method
cpg	711.79	J/mol×K	1051.68	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299664&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
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature