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

Inchi: InChI=1S/C11H12FNO3/c1-7(11(15)16-2)13-10(14)8-4-3-5-9(12)6-8/h3-7H,1-2H3,(H,13,
InchiKey: PDVYKTYSCACORC-UHFFFAOYSA-N
Formula: C11H12FNO3
SMILES: COC(=O)C(C)NC(=O)c1cccc(F)c1
Mol. weight [g/mol]: 225.22

Physical Properties

Property code	Value	Unit	Source
hfus	26.94	kJ/mol	Joback Method
ie	8.94	eV	Cheméo Relay (1.0)
logp	1.117		Crippen Method
mcvol	162.850	ml/mol	McGowan Method
rinpol	1616.00		NIST Webbook
rinpol	1616.00		NIST Webbook
tb	551.10	K	Cheméo Relay (1.0)
tf	343.80	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	419.95	J/mol×K	661.90	Joback Method
cpg	432.27	J/mol×K	697.18	Joback Method
cpg	443.78	J/mol×K	732.45	Joback Method
cpg	454.49	J/mol×K	767.73	Joback Method
cpg	464.42	J/mol×K	803.00	Joback Method
cpg	473.58	J/mol×K	838.28	Joback Method
cpg	482.00	J/mol×K	873.55	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U299674&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
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

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