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
gf	-326.18	kJ/mol	Joback Method
hf	-550.61	kJ/mol	Joback Method
hfus	26.94	kJ/mol	Joback Method
hvap	64.15	kJ/mol	Joback Method
log10ws	-2.38		Crippen Method
logp	1.117		Crippen Method
mcvol	162.850	ml/mol	McGowan Method
pc	2850.52	kPa	Joback Method
rinpol	1616.00		NIST Webbook
rinpol	1616.00		NIST Webbook
tb	661.90	K	Joback Method
tc	873.55	K	Joback Method
tf	413.01	K	Joback Method
vc	0.621	m3/kmol	Joback Method

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

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=U299674&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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