l-Alanine, N-(2,6-difluorobenzoyl)-, methyl ester

Inchi: InChI=1S/C11H11F2NO3/c1-6(11(16)17-2)14-10(15)9-7(12)4-3-5-8(9)13/h3-6H,1-2H3,(H

InchiKey: SGUFQMWTZUKVFS-UHFFFAOYSA-N

Formula: C11H11F2NO3

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

Mol. weight [g/mol]: 243.21

Physical Properties

Property code	Value	Unit	Source
gf	-530.62	kJ/mol	Joback Method
hf	-758.19	kJ/mol	Joback Method
hfus	29.63	kJ/mol	Joback Method
hvap	64.00	kJ/mol	Joback Method
log10ws	-2.71		Crippen Method
logp	1.256		Crippen Method
mcvol	164.620	ml/mol	McGowan Method
pc	2676.31	kPa	Joback Method
rinpol	1612.00		NIST Webbook
rinpol	1612.00		NIST Webbook
tb	666.15	K	Joback Method
tc	869.90	K	Joback Method
tf	426.12	K	Joback Method
vc	0.638	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	426.86	J/mol×K	666.15	Joback Method
cpg	438.45	J/mol×K	700.11	Joback Method
cpg	449.31	J/mol×K	734.07	Joback Method
cpg	459.45	J/mol×K	768.03	Joback Method
cpg	468.89	J/mol×K	801.99	Joback Method
cpg	477.63	J/mol×K	835.94	Joback Method
cpg	485.68	J/mol×K	869.90	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299660&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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