l-Alanine, N-(2,3,4-trifluorobenzoyl)-, methyl ester

Inchi: InChI=1S/C11H10F3NO3/c1-5(11(17)18-2)15-10(16)6-3-4-7(12)9(14)8(6)13/h3-5H,1-2H

InchiKey: KFBYUEGNZKBZGI-UHFFFAOYSA-N

Formula: C11H10F3NO3

SMILES: COC(=O)C(C)NC(=O)c1ccc(F)c(F)c1F

Mol. weight [g/mol]: 261.20

Physical Properties

Property code	Value	Unit	Source
gf	-735.06	kJ/mol	Joback Method
hf	-965.77	kJ/mol	Joback Method
hfus	32.32	kJ/mol	Joback Method
hvap	63.84	kJ/mol	Joback Method
log10ws	-3.04		Crippen Method
logp	1.395		Crippen Method
mcvol	166.390	ml/mol	McGowan Method
pc	2517.59	kPa	Joback Method
rinpol	1548.00		NIST Webbook
rinpol	1548.00		NIST Webbook
tb	670.40	K	Joback Method
tc	866.99	K	Joback Method
tf	439.23	K	Joback Method
vc	0.656	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	433.70	J/mol×K	670.40	Joback Method
cpg	444.63	J/mol×K	703.16	Joback Method
cpg	454.91	J/mol×K	735.93	Joback Method
cpg	464.53	J/mol×K	768.69	Joback Method
cpg	473.50	J/mol×K	801.46	Joback Method
cpg	481.84	J/mol×K	834.22	Joback Method
cpg	489.53	J/mol×K	866.99	Joback Method

Sources

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=U299627&Units=SI
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
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