l-Alanine, N-(3-trifluoromethylbenzoyl)-, methyl ester

Inchi: InChI=1S/C12H12F3NO3/c1-7(11(18)19-2)16-10(17)8-4-3-5-9(6-8)12(13,14)15/h3-7H,1-

InchiKey: OFYKTKICXHHTMS-UHFFFAOYSA-N

Formula: C12H12F3NO3

SMILES: COC(=O)C(C)NC(=O)c1cccc(C(F)(F)F)c1

Mol. weight [g/mol]: 275.22

Physical Properties

Property code	Value	Unit	Source
gf	-704.54	kJ/mol	Joback Method
hf	-972.22	kJ/mol	Joback Method
hfus	28.28	kJ/mol	Joback Method
hvap	63.45	kJ/mol	Joback Method
log10ws	-3.15		Crippen Method
logp	1.997		Crippen Method
mcvol	180.480	ml/mol	McGowan Method
pc	2402.92	kPa	Joback Method
rinpol	1594.00		NIST Webbook
tb	680.09	K	Joback Method
tc	882.17	K	Joback Method
tf	427.88	K	Joback Method
vc	0.702	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	489.51	J/mol×K	680.09	Joback Method
cpg	501.62	J/mol×K	713.77	Joback Method
cpg	512.87	J/mol×K	747.45	Joback Method
cpg	523.30	J/mol×K	781.13	Joback Method
cpg	532.95	J/mol×K	814.81	Joback Method
cpg	541.84	J/mol×K	848.49	Joback Method
cpg	550.01	J/mol×K	882.17	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=U299698&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