

L-Alanine, N-(2-trifluoromethylbenzoyl)-, methyl ester

Inchi:	InChI=1S/C12H12F3NO3/c1-7(11(18)19-2)16-10(17)8-5-3-4-6-9(8)12(13,14)15/h3-7H,1-
InchiKey:	HOYZGOAJCOOKFM-UHFFFAOYSA-N
Formula:	C12H12F3NO3
SMILES:	COC(=O)C(C)NC(=O)c1ccccc1C(F)(F)F
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
rinqol	1597.00		NIST Webbook
tb	680.09	K	Joback Method
tc	882.17	K	Joback Method
tf	427.88	K	Joback Method
vc	0.702	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299683&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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