

L-Alanine, N-(trifluoroacetyl)-, butyl ester

Other names:	Alanine, N-(trifluoroacetyl)-, butyl ester, L-Butyl N-(trifluoroacetyl)alaninate Ala, butyl ester, TFA Ala TFA Bu
Inchi:	InChI=1S/C9H14F3NO3/c1-3-4-5-16-7(14)6(2)13-8(15)9(10,11)12/h6H,3-5H2,1-2H3,(H,1
InchiKey:	MLQQWGSMDWLMKV-UHFFFAOYSA-N
Formula:	C9H14F3NO3
SMILES:	CCCCOC(=O)C(C)NC(=O)C(F)(F)F
Mol. weight [g/mol]:	241.21
CAS:	2505-26-2

Physical Properties

Property code	Value	Unit	Source
gf	-832.58	kJ/mol	Joback Method
hf	-1135.36	kJ/mol	Joback Method
hfus	26.85	kJ/mol	Joback Method
hvap	53.83	kJ/mol	Joback Method
log10ws	-2.19		Crippen Method
logp	1.397		Crippen Method
mcvol	161.970	ml/mol	McGowan Method
pc	2338.29	kPa	Joback Method
rinpol	1159.00		NIST Webbook
tb	579.79	K	Joback Method
tc	754.06	K	Joback Method
tf	355.13	K	Joback Method
vc	0.641	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	421.06	J/molxK	579.79	Joback Method
cpg	432.98	J/molxK	608.84	Joback Method
cpg	444.28	J/molxK	637.88	Joback Method
cpg	454.97	J/molxK	666.93	Joback Method

cpg	465.09	J/mol×K	695.97	Joback Method
cpg	474.63	J/mol×K	725.02	Joback Method
cpg	483.63	J/mol×K	754.06	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=C2505262&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
mvol:	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

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