Alanine, 2-methyl-N-(trifluoroacetyl)-, butyl ester

Other names: Butyl N-(trifluoroacetyl)-«alpha»-aminoisobutyrate
Butyl 2-methyl-2-[(trifluoroacetyl)amino]propanoate
Propanoic acid, 2-amino-2-methyl, butyl ester, TFA

Inchi: InChI=1S/C10H16F3NO3/c1-4-5-6-17-8(16)9(2,3)14-7(15)10(11,12)13/h4-6H2,1-3H3,(H,

InchiKey: YWDQJPHFSPNTCF-UHFFFAOYSA-N

Formula: C10H16F3NO3

SMILES: CCCCOC(=O)C(C)(C)NC(=O)C(F)(F)F

Mol. weight [g/mol]: 255.23

CAS: 34815-07-1

Physical Properties

Property code	Value	Unit	Source
gf	-818.88	kJ/mol	Joback Method
hf	-1159.47	kJ/mol	Joback Method
hfus	25.55	kJ/mol	Joback Method
hvap	55.15	kJ/mol	Joback Method
log10ws	-2.61		Crippen Method
logp	1.787		Crippen Method
mcvol	176.060	ml/mol	McGowan Method
pc	2157.31	kPa	Joback Method
rinpol	1235.00		NIST Webbook
tb	599.88	K	Joback Method
tc	778.26	K	Joback Method
tf	383.82	K	Joback Method
vc	0.693	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	472.54	J/mol×K	599.88	Joback Method
cpg	485.38	J/mol×K	629.61	Joback Method
cpg	497.46	J/mol×K	659.34	Joback Method
cpg	508.83	J/mol×K	689.07	Joback Method
cpg	519.51	J/mol×K	718.80	Joback Method

cpg	529.54	J/mol×K	748.53	Joback Method
cpg	538.95	J/mol×K	778.26	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C34815071&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