

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

Other names:	Phe, butyl ester, TFA Phe, TFA, butyl ester Alanine, 3-phenyl-N-(trifluoroacetyl)-, butyl ester, L- Phe TFA Bu
Inchi:	InChI=1S/C15H18F3NO3/c1-2-3-9-22-13(20)12(19-14(21)15(16,17)18)10-11-7-5-4-6-8-1
InchiKey:	APGGCCFPMAPWKS-UHFFFAOYSA-N
Formula:	C15H18F3NO3
SMILES:	CCCCOC(=O)C(Cc1ccccc1)NC(=O)C(F)(F)F
Mol. weight [g/mol]:	317.30
CAS:	52574-47-7

Physical Properties

Property code	Value	Unit	Source
gf	-669.65	kJ/mol	Joback Method
hf	-1022.67	kJ/mol	Joback Method
hfus	36.43	kJ/mol	Joback Method
hvap	69.46	kJ/mol	Joback Method
log10ws	-3.81		Crippen Method
logp	2.620		Crippen Method
mcvol	222.750	ml/mol	McGowan Method
pc	1869.17	kPa	Joback Method
rinpol	1678.00		NIST Webbook
rinpol	1678.00		NIST Webbook
tb	743.75	K	Joback Method
tc	939.57	K	Joback Method
tf	449.17	K	Joback Method
vc	0.870	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	648.43	J/mol×K	743.75	Joback Method
cpg	661.88	J/mol×K	776.39	Joback Method
cpg	674.40	J/mol×K	809.02	Joback Method

cpg	686.03	J/mol×K	841.66	Joback Method
cpg	696.82	J/mol×K	874.29	Joback Method
cpg	706.80	J/mol×K	906.93	Joback Method
cpg	716.04	J/mol×K	939.57	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C52574477&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

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