

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

Other names:	Norleu, butyl ester, TFA Norleu, butyl ester, N-TFA
Inchi:	InChI=1S/C12H20F3NO3/c1-3-5-7-9(10(17)19-8-6-4-2)16-11(18)12(13,14)15/h9H,3-8H2
InchiKey:	BFNUVLVKIQRVPV-SECBINFHSA-N
Formula:	C12H20F3NO3
SMILES:	CCCCOC(=O)C(CCCC)NC(=O)C(F)(F)F
Mol. weight [g/mol]:	283.29
CAS:	55044-47-8

Physical Properties

Property code	Value	Unit	Source
gf	-807.32	kJ/mol	Joback Method
hf	-1197.28	kJ/mol	Joback Method
hfus	34.62	kJ/mol	Joback Method
hvap	60.51	kJ/mol	Joback Method
log10ws	-3.45		Crippen Method
logp	2.567		Crippen Method
mcvol	204.240	ml/mol	McGowan Method
pc	1801.56	kPa	Joback Method
rinpol	1389.00		NIST Webbook
rinpol	1389.00		NIST Webbook
tb	648.43	K	Joback Method
tc	820.28	K	Joback Method
tf	388.94	K	Joback Method
vc	0.809	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	571.42	J/molxK	648.43	Joback Method
cpg	585.08	J/molxK	677.07	Joback Method
cpg	598.02	J/molxK	705.71	Joback Method
cpg	610.27	J/molxK	734.36	Joback Method
cpg	621.86	J/molxK	763.00	Joback Method

cpg	632.81	J/mol×K	791.64	Joback Method
cpg	643.13	J/mol×K	820.28	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55044478&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

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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