

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

Other names:	Isoleucine, N-(trifluoroacetyl)-, butyl ester, L Ile, butyl ester, TFA Ile TFA Bu
Inchi:	InChI=1S/C12H20F3NO3/c1-4-6-7-19-10(17)9(8(3)5-2)16-11(18)12(13,14)15/h8-9H,4-7H
InchiKey:	RXCCQFOMEQOSMR-RKDXNWHRSA-N
Formula:	C12H20F3NO3
SMILES:	CCCCOC(=O)C(NC(=O)C(F)(F)F)C(C)CC
Mol. weight [g/mol]:	283.29
CAS:	2505-28-4

Physical Properties

Property code	Value	Unit	Source
gf	-809.76	kJ/mol	Joback Method
hf	-1202.56	kJ/mol	Joback Method
hfus	31.10	kJ/mol	Joback Method
hvap	60.12	kJ/mol	Joback Method
log10ws	-3.21		Crippen Method
logp	2.423		Crippen Method
mcvol	204.240	ml/mol	McGowan Method
pc	1813.86	kPa	Joback Method
rinpola	1358.00		NIST Webbook
rinpola	1358.00		NIST Webbook
tb	647.99	K	Joback Method
tc	822.24	K	Joback Method
tf	373.94	K	Joback Method
vc	0.803	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	571.88	J/molxK	647.99	Joback Method
cpg	585.76	J/molxK	677.03	Joback Method
cpg	598.90	J/molxK	706.07	Joback Method
cpg	611.33	J/molxK	735.12	Joback Method

cpg	623.07	J/mol×K	764.16	Joback Method
cpg	634.13	J/mol×K	793.20	Joback Method
cpg	644.55	J/mol×K	822.24	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2505284&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

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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