

I-Leucine, N-ethoxycarbonyl-N-methyl-, octyl ester

Inchi:	InChI=1S/C18H35NO4/c1-6-8-9-10-11-12-13-23-17(20)16(14-15(3)4)19(5)18(21)22-7-2/
InchiKey:	JDWPAESHZQQJEL-UHFFFAOYSA-N
Formula:	C18H35NO4
SMILES:	CCCCCCCCOC(=O)C(CC(C)C)N(C)C(=O)OCC
Mol. weight [g/mol]:	329.47

Physical Properties

Property code	Value	Unit	Source
gf	-261.26	kJ/mol	Joback Method
hf	-847.48	kJ/mol	Joback Method
hfus	43.92	kJ/mol	Joback Method
hvap	75.24	kJ/mol	Joback Method
log10ws	-4.50		Crippen Method
logp	4.393		Crippen Method
mcvol	289.340	ml/mol	McGowan Method
pc	1239.83	kPa	Joback Method
rinsol	2034.00		NIST Webbook
tb	775.38	K	Joback Method
tc	957.28	K	Joback Method
tf	439.41	K	Joback Method
vc	1.097	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	892.99	J/molxK	775.38	Joback Method
cpg	910.82	J/molxK	805.70	Joback Method
cpg	927.65	J/molxK	836.01	Joback Method
cpg	943.49	J/molxK	866.33	Joback Method
cpg	958.38	J/molxK	896.65	Joback Method
cpg	972.31	J/molxK	926.96	Joback Method
cpg	985.32	J/molxK	957.28	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=U321924&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccol:	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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