

I-Leucine, N-isobutoxycarbonyl-N-methyl-, nonyl ester

Inchi:	InChI=1S/C21H41NO4/c1-7-8-9-10-11-12-13-14-25-20(23)19(15-17(2)3)22(6)21(24)26-1
InchiKey:	VPKCGZNXNDUMFX-UHFFFAOYSA-N
Formula:	C21H41NO4
SMILES:	CCCCCCCCCOC(=O)C(CC(C)C)N(C)C(=O)OCC(C)C
Mol. weight [g/mol]:	371.55

Physical Properties

Property code	Value	Unit	Source
gf	-238.44	kJ/mol	Joback Method
hf	-914.68	kJ/mol	Joback Method
hfus	48.17	kJ/mol	Joback Method
hvap	81.53	kJ/mol	Joback Method
log10ws	-5.51		Crippen Method
logp	5.419		Crippen Method
mvol	331.610	ml/mol	McGowan Method
pc	1027.28	kPa	Joback Method
rinpol	2245.00		NIST Webbook
tb	843.58	K	Joback Method
tc	1034.17	K	Joback Method
tf	458.22	K	Joback Method
vc	1.260	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1075.42	J/mol×K	843.58	Joback Method
cpg	1094.38	J/mol×K	875.35	Joback Method
cpg	1112.13	J/mol×K	907.11	Joback Method
cpg	1128.71	J/mol×K	938.88	Joback Method
cpg	1144.15	J/mol×K	970.64	Joback Method
cpg	1158.47	J/mol×K	1002.41	Joback Method
cpg	1171.70	J/mol×K	1034.17	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321875&Units=SI

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
h vap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m cvol:	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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