

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

Inchi:	InChI=1S/C20H37NO4/c1-6-8-9-10-11-12-13-15-24-19(22)18(16-17(3)4)21(5)20(23)25-1
InchiKey:	XGZRBEDPZINOIA-UHFFFAOYSA-N
Formula:	C20H37NO4
SMILES:	C=CCOC(=O)N(C)C(CC(C)C)C(=O)OCCCCCCCCC
Mol. weight [g/mol]:	355.51

Physical Properties

Property code	Value	Unit	Source
gf	-156.58	kJ/mol	Joback Method
hf	-763.33	kJ/mol	Joback Method
hfus	47.82	kJ/mol	Joback Method
hvap	79.02	kJ/mol	Joback Method
log10ws	-5.19		Crippen Method
logp	4.949		Crippen Method
mcvol	313.220	ml/mol	McGowan Method
pc	1118.56	kPa	Joback Method
rinpol	2192.00		NIST Webbook
tb	817.82	K	Joback Method
tc	1004.78	K	Joback Method
tf	460.19	K	Joback Method
vc	1.190	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	986.33	J/molxK	817.82	Joback Method
cpg	1004.33	J/molxK	848.98	Joback Method
cpg	1021.26	J/molxK	880.14	Joback Method
cpg	1037.13	J/molxK	911.30	Joback Method
cpg	1051.97	J/molxK	942.46	Joback Method
cpg	1065.82	J/molxK	973.62	Joback Method
cpg	1078.69	J/molxK	1004.78	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=U321902&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
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	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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