

I-Leucine, N-methyl-n-propoxycarbonyl-, nonyl ester

Inchi:	InChI=1S/C20H39NO4/c1-6-8-9-10-11-12-13-15-24-19(22)18(16-17(3)4)21(5)20(23)25-1
InchiKey:	ILLCTVFGWJWSAW-UHFFFAOYSA-N
Formula:	C20H39NO4
SMILES:	CCCCCCCCCOC(=O)C(CC(C)C)N(C)C(=O)OCCC
Mol. weight [g/mol]:	357.53

Physical Properties

Property code	Value	Unit	Source
gf	-244.42	kJ/mol	Joback Method
hf	-888.76	kJ/mol	Joback Method
hfus	49.10	kJ/mol	Joback Method
hvap	79.69	kJ/mol	Joback Method
log10ws	-5.34		Crippen Method
logp	5.173		Crippen Method
mvol	317.520	ml/mol	McGowan Method
pc	1087.78	kPa	Joback Method
rinpol	2197.00		NIST Webbook
rinpol	2197.00		NIST Webbook
tb	821.14	K	Joback Method
tc	1007.78	K	Joback Method
tf	461.95	K	Joback Method
vc	1.210	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1013.53	J/mol×K	821.14	Joback Method
cpg	1032.07	J/mol×K	852.25	Joback Method
cpg	1049.49	J/mol×K	883.35	Joback Method
cpg	1065.82	J/mol×K	914.46	Joback Method
cpg	1081.08	J/mol×K	945.57	Joback Method
cpg	1095.30	J/mol×K	976.68	Joback Method
cpg	1108.50	J/mol×K	1007.78	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321859&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
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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