

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

Inchi:	InChI=1S/C21H39NO4/c1-6-8-9-10-11-12-13-14-16-25-20(23)19(17-18(3)4)22(5)21(24)2
InchiKey:	BHXGSAWPBAINEW-UHFFFAOYSA-N
Formula:	C21H39NO4
SMILES:	C=CCOC(=O)N(C)C(CC(C)C)C(=O)OCCCCCCCCC
Mol. weight [g/mol]:	369.54

Physical Properties

Property code	Value	Unit	Source
gf	-148.16	kJ/mol	Joback Method
hf	-783.97	kJ/mol	Joback Method
hfus	50.41	kJ/mol	Joback Method
hvap	81.25	kJ/mol	Joback Method
log10ws	-5.61		Crippen Method
logp	5.339		Crippen Method
mcvol	327.310	ml/mol	McGowan Method
pc	1050.05	kPa	Joback Method
rinpol	2297.00		NIST Webbook
rinpol	2297.00		NIST Webbook
tb	840.70	K	Joback Method
tc	1030.77	K	Joback Method
tf	471.46	K	Joback Method
vc	1.246	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1047.23	J/molxK	840.70	Joback Method
cpg	1065.61	J/molxK	872.38	Joback Method
cpg	1082.84	J/molxK	904.06	Joback Method
cpg	1098.96	J/molxK	935.74	Joback Method
cpg	1114.00	J/molxK	967.41	Joback Method
cpg	1127.99	J/molxK	999.09	Joback Method
cpg	1140.96	J/molxK	1030.77	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=U321903&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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