

I-Leucine, N-neopentylloxycarbonyl-N-methyl-, heptadecyl ester

Inchi:	InChI=1S/C30H59NO4/c1-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-34-28(32)27
InchiKey:	IFBBUSKNSJPIML-UHFFFAOYSA-N
Formula:	C30H59NO4
SMILES:	CCCCCCCCCCCCCCCCOC(=O)C(CC(C)C)N(C)C(=O)OCC(C)(C)C
Mol. weight [g/mol]:	497.79

Physical Properties

Property code	Value	Unit	Source
gf	-157.38	kJ/mol	Joback Method
hf	-1103.91	kJ/mol	Joback Method
hfus	67.59	kJ/mol	Joback Method
hvap	100.66	kJ/mol	Joback Method
log10ws	-9.28		Crippen Method
logp	8.930		Crippen Method
mvol	458.420	ml/mol	McGowan Method
pc	633.52	kPa	Joback Method
rinpol	3261.00		NIST Webbook
rinpol	3261.00		NIST Webbook
tb	1046.71	K	Joback Method
tc	1305.41	K	Joback Method
tf	577.07	K	Joback Method
vc	1.758	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1650.83	J/molxK	1046.71	Joback Method
cpg	1674.45	J/molxK	1089.83	Joback Method
cpg	1695.93	J/molxK	1132.94	Joback Method
cpg	1715.44	J/molxK	1176.06	Joback Method
cpg	1733.14	J/molxK	1219.18	Joback Method
cpg	1749.19	J/molxK	1262.29	Joback Method
cpg	1763.73	J/molxK	1305.41	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=U321918&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
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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