

L-Leucine, N-ethoxycarbonyl-N-methyl-, pentadecyl ester

Inchi: InChI=1S/C25H49NO4/c1-6-8-9-10-11-12-13-14-15-16-17-18-19-20-30-24(27)23(21-22(30)25)26
InchiKey: FWZCAARLHWGSOM-UHFFFAOYSA-N
Formula: C25H49NO4
SMILES: CCCCCCCCCCCCCCCCCOC(=O)C(CC(C)C)N(C)C(=O)OCC
Mol. weight [g/mol]: 427.67

Physical Properties

Property code	Value	Unit	Source
hf	-1134.62	kJ/mol	Cheméo Relay (1.0)
hfus	62.05	kJ/mol	Joback Method
hvap	121.89	kJ/mol	Cheméo Relay (1.0)
log10ws	-6.47		Cheméo Relay (1.0)
logp	7.124		Crippen Method
mcvol	387.970	ml/mol	McGowan Method
rinpol	2725.00		NIST Webbook
tb	646.47	K	Cheméo Relay (1.0)
tf	285.32	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1326.77	J/mol×K	935.54	Joback Method
cpg	1347.53	J/mol×K	971.09	Joback Method
cpg	1366.71	J/mol×K	1006.64	Joback Method
cpg	1384.35	J/mol×K	1042.19	Joback Method
cpg	1400.51	J/mol×K	1077.74	Joback Method
cpg	1415.24	J/mol×K	1113.29	Joback Method
cpg	1428.60	J/mol×K	1148.84	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321929&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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