L-leucine, n-isobutoxycarbonyl-n-methyl-, pentadecyl ester

Inchi: InChI=1S/C27H53NO4/c1-7-8-9-10-11-12-13-14-15-16-17-18-19-20-31-26(29)25(21-23(2

InchiKey: IEDXANWFKHOIMY-UHFFFAOYSA-N

Formula: C27H53NO4

SMILES: CCCCCCCCCCCCCCCCOC(=O)C(CC(C)C)N(C)C(=O)OCC(C)C

Mol. weight [g/mol]: 455.72

Physical Properties

Property code	Value	Unit	Source
hf	-1186.76	kJ/mol	Cheméo Relay (1.0)
hfus	63.71	kJ/mol	Joback Method
hvap	122.70	kJ/mol	Cheméo Relay (1.0)
log10ws	-7.05		Cheméo Relay (1.0)
logp	7.760		Crippen Method
mcvol	416.150	ml/mol	McGowan Method
rinpol	2879.00		NIST Webbook
rinpol	2879.00		NIST Webbook
tb	660.42	K	Cheméo Relay (1.0)
tf	284.50	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1455.86	J/mol×K	980.86	Joback Method
cpg	1477.58	J/mol×K	1019.11	Joback Method
cpg	1497.41	J/mol×K	1057.37	Joback Method
cpg	1515.45	J/mol×K	1095.62	Joback Method
cpg	1531.76	J/mol×K	1133.87	Joback Method
cpg	1546.42	J/mol×K	1172.13	Joback Method
cpg	1559.49	J/mol×K	1210.38	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=U321878&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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