L-Leucine, N-methyl-N-(2-ethylhexyloxycarbonyl)-, 2-ethylhexyl ester

Inchi: InChI=1S/C24H47NO4/c1-8-12-14-20(10-3)17-28-23(26)22(16-19(5)6)25(7)24(27)29-18-
InchiKey: GUQMKWFYHFXPES-UHFFFAOYSA-N
Formula: C24H47NO4
SMILES: CCCCC(CC)COC(=O)C(CC(C)C)N(C)C(=O)OCC(CC)CCCC
Mol. weight [g/mol]: 413.63

Physical Properties

Property code	Value	Unit	Source
gf	-215.62	kJ/mol	Joback Method
hf	-981.88	kJ/mol	Joback Method
hfus	52.42	kJ/mol	Joback Method
hvap	87.82	kJ/mol	Joback Method
log10ws	-6.53		Crippen Method
logp	6.446		Crippen Method
mcvol	373.880	ml/mol	McGowan Method
pc	865.05	kPa	Joback Method
rinpol	2344.00		NIST Webbook
rinpol	2344.00		NIST Webbook
tb	911.78	K	Joback Method
tc	1116.63	K	Joback Method
tf	477.03	K	Joback Method
vc	1.421	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1263.83	J/mol×K	911.78	Joback Method
cpg	1283.92	J/mol×K	945.92	Joback Method
cpg	1302.53	J/mol×K	980.06	Joback Method
cpg	1319.71	J/mol×K	1014.21	Joback Method
cpg	1335.51	J/mol×K	1048.35	Joback Method
cpg	1349.97	J/mol×K	1082.49	Joback Method
cpg	1363.13	J/mol×K	1116.63	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=U392397&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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