DL-Valine, N-methyl-N-(2-ethylhexyloxycarbonyl)-, decyl ester

Inchi: InChI=1S/C25H49NO4/c1-7-10-12-13-14-15-16-17-19-29-24(27)23(21(4)5)26(6)25(28)30
InchiKey: QYSJHHSLJUGIEJ-UHFFFAOYSA-N
Formula: C25H49NO4
SMILES: CCCCCCCCCCOC(=O)C(C(C)C)N(C)C(=O)OCC(CC)CCCC
Mol. weight [g/mol]: 427.66

Physical Properties

Property code	Value	Unit	Source
gf	-204.76	kJ/mol	Joback Method
hf	-997.24	kJ/mol	Joback Method
hfus	58.53	kJ/mol	Joback Method
hvap	90.43	kJ/mol	Joback Method
log10ws	-7.19		Crippen Method
logp	6.980		Crippen Method
mcvol	387.970	ml/mol	McGowan Method
pc	814.46	kPa	Joback Method
rinpol	2623.00		NIST Webbook
rinpol	2623.00		NIST Webbook
tb	935.10	K	Joback Method
tc	1147.35	K	Joback Method
tf	503.30	K	Joback Method
vc	1.484	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1327.15	J/mol×K	935.10	Joback Method
cpg	1347.78	J/mol×K	970.48	Joback Method
cpg	1366.83	J/mol×K	1005.85	Joback Method
cpg	1384.34	J/mol×K	1041.23	Joback Method
cpg	1400.37	J/mol×K	1076.60	Joback Method
cpg	1414.98	J/mol×K	1111.98	Joback Method
cpg	1428.21	J/mol×K	1147.35	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392914&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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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