l-Norvaline, N-isobutoxycarbonyl-, dodecyl ester

Inchi: InChI=1S/C22H43NO4/c1-5-7-8-9-10-11-12-13-14-15-17-26-21(24)20(16-6-2)23-22(25)2

InchiKey: NEXRNOCUCGOTJA-UHFFFAOYSA-N

Formula: C22H43NO4

SMILES: CCCCCCCCCCCCOC(=O)C(CCC)NC(=O)OCC(C)C

Mol. weight [g/mol]: 385.58

Physical Properties

Property code	Value	Unit	Source
gf	-248.97	kJ/mol	Joback Method
hf	-944.10	kJ/mol	Joback Method
hfus	56.36	kJ/mol	Joback Method
hvap	88.54	kJ/mol	Joback Method
log10ws	-6.79		Crippen Method
logp	6.001		Crippen Method
mcvol	345.700	ml/mol	McGowan Method
pc	971.09	kPa	Joback Method
rinpol	2271.00		NIST Webbook
tb	904.63	K	Joback Method
tc	1107.67	K	Joback Method
tf	504.68	K	Joback Method
vc	1.339	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1158.20	J/mol×K	904.63	Joback Method
cpg	1176.86	J/mol×K	938.47	Joback Method
cpg	1194.17	J/mol×K	972.31	Joback Method
cpg	1210.14	J/mol×K	1006.15	Joback Method
cpg	1224.81	J/mol×K	1039.99	Joback Method
cpg	1238.20	J/mol×K	1073.83	Joback Method
cpg	1250.35	J/mol×K	1107.67	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320721&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
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