l-Norvaline, N-ethoxycarbonyl-, isohexyl ester

Inchi: InChI=1S/C14H27NO4/c1-5-8-12(15-14(17)18-6-2)13(16)19-10-7-9-11(3)4/h11-12H,5-10
InchiKey: LDLKTQPBJBFNBN-UHFFFAOYSA-N
Formula: C14H27NO4
SMILES: CCCC(NC(=O)OCC)C(=O)OCCCC(C)C
Mol. weight [g/mol]: 273.37

Physical Properties

Property code	Value	Unit	Source
gf	-316.33	kJ/mol	Joback Method
hf	-778.98	kJ/mol	Joback Method
hfus	35.64	kJ/mol	Joback Method
hvap	70.73	kJ/mol	Joback Method
log10ws	-3.45		Crippen Method
logp	2.881		Crippen Method
mcvol	232.980	ml/mol	McGowan Method
pc	1678.28	kPa	Joback Method
rinpol	1630.00		NIST Webbook
rinpol	1630.00		NIST Webbook
tb	721.59	K	Joback Method
tc	905.40	K	Joback Method
tf	414.52	K	Joback Method
vc	0.890	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	681.95	J/mol×K	721.59	Joback Method
cpg	697.70	J/mol×K	752.23	Joback Method
cpg	712.60	J/mol×K	782.86	Joback Method
cpg	726.66	J/mol×K	813.50	Joback Method
cpg	739.90	J/mol×K	844.13	Joback Method
cpg	752.31	J/mol×K	874.77	Joback Method
cpg	763.90	J/mol×K	905.40	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320702&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