l-Norvaline, N-isobutoxycarbonyl-, isohexyl ester

Inchi: InChI=1S/C16H31NO4/c1-6-8-14(17-16(19)21-11-13(4)5)15(18)20-10-7-9-12(2)3/h12-14

InchiKey: QNFGEQCXAQCBCN-UHFFFAOYSA-N

Formula: C16H31NO4

SMILES: CCCC(NC(=O)OCC(C)C)C(=O)OCCCC(C)C

Mol. weight [g/mol]: 301.42

Physical Properties

Property code	Value	Unit	Source
gf	-301.93	kJ/mol	Joback Method
hf	-825.54	kJ/mol	Joback Method
hfus	37.30	kJ/mol	Joback Method
hvap	74.79	kJ/mol	Joback Method
log10ws	-4.04		Crippen Method
logp	3.517		Crippen Method
mcvol	261.160	ml/mol	McGowan Method
pc	1451.25	kPa	Joback Method
rinpol	1737.00		NIST Webbook
rinpol	1737.00		NIST Webbook
tb	766.91	K	Joback Method
tc	953.11	K	Joback Method
tf	422.06	K	Joback Method
vc	0.997	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	796.33	J/mol×K	766.91	Joback Method
cpg	812.99	J/mol×K	797.94	Joback Method
cpg	828.68	J/mol×K	828.98	Joback Method
cpg	843.41	J/mol×K	860.01	Joback Method
cpg	857.20	J/mol×K	891.04	Joback Method
cpg	870.07	J/mol×K	922.08	Joback Method
cpg	882.01	J/mol×K	953.11	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=U320716&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