L-Norvaline, N-hexyloxycarbonyl-, isobutyl ester

Inchi: InChI=1S/C16H31NO4/c1-5-7-8-9-11-20-16(19)17-14(10-6-2)15(18)21-12-13(3)4/h13-14
InchiKey: RASRTLAPFQGSOF-CQSZACIVSA-N
Formula: C16H31NO4
SMILES: CCCCCCOC(=O)NC(CCC)C(=O)OCC(C)C
Mol. weight [g/mol]: 301.42

Physical Properties

Property code	Value	Unit	Source
gf	-299.49	kJ/mol	Joback Method
hf	-820.26	kJ/mol	Joback Method
hfus	40.82	kJ/mol	Joback Method
hvap	75.18	kJ/mol	Joback Method
log10ws	-4.28		Crippen Method
logp	3.661		Crippen Method
mcvol	261.160	ml/mol	McGowan Method
pc	1442.44	kPa	Joback Method
rinpol	1978.00		NIST Webbook
rinpol	1978.00		NIST Webbook
tb	767.35	K	Joback Method
tc	951.81	K	Joback Method
tf	437.06	K	Joback Method
vc	1.002	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	795.83	J/mol×K	767.35	Joback Method
cpg	812.32	J/mol×K	798.09	Joback Method
cpg	827.87	J/mol×K	828.84	Joback Method
cpg	842.49	J/mol×K	859.58	Joback Method
cpg	856.20	J/mol×K	890.33	Joback Method
cpg	869.00	J/mol×K	921.07	Joback Method
cpg	880.90	J/mol×K	951.81	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=U392831&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