l-Norvaline, N-isobutoxycarbonyl-, octadecyl ester

Inchi: InChI=1S/C28H55NO4/c1-5-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-23-32-27(30)26

InchiKey: HIYSYWYNYUODIU-UHFFFAOYSA-N

Formula: C28H55NO4

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

Mol. weight [g/mol]: 469.74

Physical Properties

Property code	Value	Unit	Source
gf	-198.45	kJ/mol	Joback Method
hf	-1067.94	kJ/mol	Joback Method
hfus	71.90	kJ/mol	Joback Method
hvap	101.89	kJ/mol	Joback Method
log10ws	-9.31		Crippen Method
logp	8.342		Crippen Method
mcvol	430.240	ml/mol	McGowan Method
pc	698.02	kPa	Joback Method
tb	1041.91	K	Joback Method
tc	1299.98	K	Joback Method
tf	572.30	K	Joback Method
vc	1.675	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1540.46	J/mol×K	1041.91	Joback Method
cpg	1562.26	J/mol×K	1084.92	Joback Method
cpg	1581.72	J/mol×K	1127.93	Joback Method
cpg	1598.94	J/mol×K	1170.95	Joback Method
cpg	1614.02	J/mol×K	1213.96	Joback Method
cpg	1627.06	J/mol×K	1256.97	Joback Method
cpg	1638.14	J/mol×K	1299.98	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=U320726&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume