l-Norvaline, N-isobutoxycarbonyl-, pentadecyl ester

Inchi: InChI=1S/C25H49NO4/c1-5-7-8-9-10-11-12-13-14-15-16-17-18-20-29-24(27)23(19-6-2)2

InchiKey: OZBXKVYDPLLJOO-UHFFFAOYSA-N

Formula: C25H49NO4

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

Mol. weight [g/mol]: 427.66

Physical Properties

Property code	Value	Unit	Source
gf	-223.71	kJ/mol	Joback Method
hf	-1006.02	kJ/mol	Joback Method
hfus	64.13	kJ/mol	Joback Method
hvap	95.22	kJ/mol	Joback Method
log10ws	-8.05		Crippen Method
logp	7.172		Crippen Method
mcvol	387.970	ml/mol	McGowan Method
pc	817.73	kPa	Joback Method
rinpol	2518.00		NIST Webbook
tb	973.27	K	Joback Method
tc	1198.16	K	Joback Method
tf	538.49	K	Joback Method
vc	1.506	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1347.62	J/mol×K	973.27	Joback Method
cpg	1367.68	J/mol×K	1010.75	Joback Method
cpg	1386.00	J/mol×K	1048.23	Joback Method
cpg	1402.62	J/mol×K	1085.72	Joback Method
cpg	1417.61	J/mol×K	1123.20	Joback Method
cpg	1431.00	J/mol×K	1160.68	Joback Method
cpg	1442.86	J/mol×K	1198.16	Joback Method

Sources

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=U320723&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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