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]: 427.67

Physical Properties

Property code	Value	Unit	Source
hf	-1184.32	kJ/mol	Cheméo Relay (1.0)
hfus	64.13	kJ/mol	Joback Method
hvap	121.89	kJ/mol	Cheméo Relay (1.0)
log10ws	-7.06		Cheméo Relay (1.0)
logp	7.172		Crippen Method
mcvol	387.970	ml/mol	McGowan Method
rinpol	2518.00		NIST Webbook
tb	645.86	K	Cheméo Relay (1.0)
tf	316.25	K	Cheméo Relay (1.0)

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

Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320723&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point