

L-Norvaline, N-isobutoxycarbonyl-, hexadecyl ester

Inchi:	InChI=1S/C26H51NO4/c1-5-7-8-9-10-11-12-13-14-15-16-17-18-19-21-30-25(28)24(20-6
InchiKey:	OFEFFOWEOYMBJC-UHFFFAOYSA-N
Formula:	C26H51NO4
SMILES:	CCCCCCCCCCCCCCCCOC(=O)C(CCC)NC(=O)OCC(C)C
Mol. weight [g/mol]:	441.70

Physical Properties

Property code	Value	Unit	Source
hf	-1203.99	kJ/mol	Cheméo Relay (1.0)
hfus	66.72	kJ/mol	Joback Method
hvap	125.78	kJ/mol	Cheméo Relay (1.0)
log10ws	-7.37		Cheméo Relay (1.0)
logp	7.562		Crippen Method
mcvol	402.060	ml/mol	McGowan Method
tb	652.56	K	Cheméo Relay (1.0)
tf	319.34	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1411.58	J/mol×K	996.15	Joback Method
cpg	1432.19	J/mol×K	1035.24	Joback Method
cpg	1450.87	J/mol×K	1074.34	Joback Method
cpg	1467.71	J/mol×K	1113.43	Joback Method
cpg	1482.76	J/mol×K	1152.52	Joback Method
cpg	1496.08	J/mol×K	1191.62	Joback Method
cpg	1507.75	J/mol×K	1230.71	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U320724&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/ci990307I>

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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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