

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)2
InchiKey:	HIYSYWYNYUODIU-UHFFFAOYSA-N
Formula:	C28H55NO4
SMILES:	CCCCCCCCCCCCCCCCCCCCOC(=O)C(CCC)NC(=O)OCC(C)C
Mol. weight [g/mol]:	469.75

Physical Properties

Property code	Value	Unit	Source
hf	-1243.81	kJ/mol	Cheméo Relay (1.0)
hfus	71.90	kJ/mol	Joback Method
hvap	133.52	kJ/mol	Cheméo Relay (1.0)
log10ws	-7.99		Cheméo Relay (1.0)
logp	8.342		Crippen Method
mcvol	430.240	ml/mol	McGowan Method
tb	665.84	K	Cheméo Relay (1.0)
tf	324.46	K	Cheméo Relay (1.0)

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U320726&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>

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

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