L-Norvaline, N-octyloxycarbonyl-, octyl ester

Inchi: InChI=1S/C22H43NO4/c1-4-7-9-11-13-15-18-26-21(24)20(17-6-3)23-22(25)27-19-16-14-

InchiKey: WYLQEZLKCDZQJM-HXUWFJFHSA-N

Formula: C22H43NO4

SMILES: CCCCCCCCOC(=O)C(CCC)N=C(O)OCCCCCCCC

Mol. weight [g/mol]: 385.58

Physical Properties

Property code	Value	Unit	Source
hf	-1105.12	kJ/mol	Cheméo Relay (1.0)
hvap	122.89	kJ/mol	Cheméo Relay (1.0)
log10ws	-5.78		Cheméo Relay (1.0)
logp	6.350		Crippen Method
mcvol	345.700	ml/mol	McGowan Method
pc	895.34	kPa	Joback Method
rinpol	2588.00		NIST Webbook
rinpol	2588.00		NIST Webbook
tb	628.48	K	Cheméo Relay (1.0)
tc	833.02	K	Cheméo Relay (1.0)
tf	316.77	K	Cheméo Relay (1.0)

Sources

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U392848&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

hf:	Enthalpy of formation 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

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