

I-Norvaline, N-isobutoxycarbonyl-, nonyl ester

Inchi: InChI=1S/C19H37NO4/c1-5-7-8-9-10-11-12-14-23-18(21)17(13-6-2)20-19(22)24-15-16(3)
InchiKey: VRXBOHLBCFTZIK-UHFFFAOYSA-N
Formula: C19H37NO4
SMILES: CCCCCCCCCOC(=O)C(CCC)N=C(O)OCC(C)C
Mol. weight [g/mol]: 343.50

Physical Properties

Property code	Value	Unit	Source
hf	-902.87	kJ/mol	Joback Method
hvap	88.75	kJ/mol	Joback Method
log10ws	-5.07		Crippen Method
logp	5.036		Crippen Method
mcvol	303.430	ml/mol	McGowan Method
pc	1107.42	kPa	Joback Method
rinpol	2029.00		NIST Webbook
rinpol	2029.00		NIST Webbook
tb	900.69	K	Joback Method
tc	1102.71	K	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=U320719&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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

Latest version available from:

<https://www.cheméo.com/cid/97-703-4/l-Norvaline-N-isobutoxycarbonyl-nonyl-ester.pdf>

Generated by Cheméo on 2024-04-27 20:19:44.516454763 +0000 UTC m=+16538433.437032076.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.