

L-Norvaline, N-methoxycarbonyl-, propyl ester

Inchi: InChI=1S/C10H19NO4/c1-4-6-8(11-10(13)14-3)9(12)15-7-5-2/h8H,4-7H2,1-3H3,(H,11,13)
InchiKey: FPVMZEKPF AHJJS-UHFFFAOYSA-N
Formula: C10H19NO4
SMILES: CCCOC(=O)C(CCC)N=C(O)OC
Mol. weight [g/mol]: 217.26

Physical Properties

Property code	Value	Unit	Source
hf	-711.83	kJ/mol	Joback Method
hvap	69.11	kJ/mol	Joback Method
log10ws	-1.55		Crippen Method
logp	1.669		Crippen Method
mcvol	176.620	ml/mol	McGowan Method
pc	2165.35	kPa	Joback Method
rinpol	1409.00		NIST Webbook
rinpol	1409.00		NIST Webbook
tb	695.21	K	Joback Method
tc	880.59	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=U320759&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

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