L-Norvaline, N-isobutoxycarbonyl-, propyl ester

Inchi: InChI=1S/C13H25NO4/c1-5-7-11(12(15)17-8-6-2)14-13(16)18-9-10(3)4/h10-11H,5-9H2,1

InchiKey: KCJVMQWUIFHMBX-UHFFFAOYSA-N

Formula: C13H25NO4

SMILES: CCCOC(=O)C(CCC)NC(=O)OCC(C)C

Mol. weight [g/mol]: 259.35

Physical Properties

Property code	Value	Unit	Source
hfus	33.05	kJ/mol	Joback Method
logp	2.491		Crippen Method
mcvol	218.890	ml/mol	McGowan Method
pc	1818.50	kPa	Joback Method
rinpol	1558.00		NIST Webbook
tb	554.71	K	Cheméo Relay (1.0)
tc	727.76	K	Cheméo Relay (1.0)
tf	272.77	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	626.67	J/mol×K	698.71	Joback Method
cpg	642.00	J/mol×K	729.42	Joback Method
cpg	656.53	J/mol×K	760.14	Joback Method
cpg	670.26	J/mol×K	790.85	Joback Method
cpg	683.21	J/mol×K	821.56	Joback Method
cpg	695.37	J/mol×K	852.27	Joback Method
cpg	706.75	J/mol×K	882.99	Joback Method

Sources

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=U320713&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
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