L-Norvaline, N-ethoxycarbonyl-, isobutyl ester

Inchi: InChI=1S/C12H23NO4/c1-5-7-10(13-12(15)16-6-2)11(14)17-8-9(3)4/h9-10H,5-8H2,1-4H3
InchiKey: BSTWGVGTAXSPHD-UHFFFAOYSA-N
Formula: C12H23NO4
SMILES: CCCC(NC(=O)OCC)C(=O)OCC(C)C
Mol. weight [g/mol]: 245.32

Physical Properties

Property code	Value	Unit	Source
hf	-934.95	kJ/mol	Cheméo Relay (1.0)
hfus	30.46	kJ/mol	Joback Method
hvap	76.58	kJ/mol	Cheméo Relay (1.0)
ie	9.02	eV	Cheméo Relay (1.0)
logp	2.100		Crippen Method
mcvol	204.800	ml/mol	McGowan Method
pc	1977.07	kPa	Joback Method
rinpol	1483.00		NIST Webbook
rinpol	1483.00		NIST Webbook
tb	542.00	K	Cheméo Relay (1.0)
tc	714.69	K	Cheméo Relay (1.0)
tf	282.50	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	572.60	J/mol×K	675.83	Joback Method
cpg	587.47	J/mol×K	706.70	Joback Method
cpg	601.58	J/mol×K	737.56	Joback Method
cpg	614.95	J/mol×K	768.43	Joback Method
cpg	627.56	J/mol×K	799.30	Joback Method
cpg	639.42	J/mol×K	830.16	Joback Method
cpg	650.54	J/mol×K	861.03	Joback Method

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=U320699&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
ie:	Ionization energy
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