l-Norvaline, n-propoxycarbonyl-, ethyl ester

Inchi: InChI=1S/C11H21NO4/c1-4-7-9(10(13)15-6-3)12-11(14)16-8-5-2/h9H,4-8H2,1-3H3,(H,12
InchiKey: SYVNMWJPDMSUSH-UHFFFAOYSA-N
Formula: C11H21NO4
SMILES: CCCOC(=O)NC(CCC)C(=O)OCC
Mol. weight [g/mol]: 231.29

Physical Properties

Property code	Value	Unit	Source
gf	-339.15	kJ/mol	Joback Method
hf	-711.78	kJ/mol	Joback Method
hfus	31.40	kJ/mol	Joback Method
hvap	64.44	kJ/mol	Joback Method
log10ws	-2.43		Crippen Method
logp	1.854		Crippen Method
mcvol	190.710	ml/mol	McGowan Method
pc	2141.36	kPa	Joback Method
rinpol	1458.00		NIST Webbook
rinpol	1458.00		NIST Webbook
tb	653.39	K	Joback Method
tc	837.00	K	Joback Method
tf	395.71	K	Joback Method
vc	0.729	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	519.38	J/mol×K	653.39	Joback Method
cpg	533.47	J/mol×K	683.99	Joback Method
cpg	546.88	J/mol×K	714.59	Joback Method
cpg	559.61	J/mol×K	745.20	Joback Method
cpg	571.67	J/mol×K	775.80	Joback Method
cpg	583.04	J/mol×K	806.40	Joback Method
cpg	593.74	J/mol×K	837.00	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320727&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion 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
vc:	Critical Volume