l-Norvaline, n-propoxycarbonyl-, pentyl ester

Inchi: InChI=1S/C14H27NO4/c1-4-7-8-11-18-13(16)12(9-5-2)15-14(17)19-10-6-3/h12H,4-11H2
InchiKey: NOHRJECQEZHVIP-UHFFFAOYSA-N
Formula: C14H27NO4
SMILES: CCCCCOC(=O)C(CCC)NC(=O)OCCC
Mol. weight [g/mol]: 273.37

Physical Properties

Property code	Value	Unit	Source
gf	-313.89	kJ/mol	Joback Method
hf	-773.70	kJ/mol	Joback Method
hfus	39.17	kJ/mol	Joback Method
hvap	71.12	kJ/mol	Joback Method
log10ws	-3.69		Crippen Method
logp	3.025		Crippen Method
mcvol	232.980	ml/mol	McGowan Method
pc	1667.33	kPa	Joback Method
rinpol	1678.00		NIST Webbook
rinpol	1678.00		NIST Webbook
tb	722.03	K	Joback Method
tc	903.69	K	Joback Method
tf	429.52	K	Joback Method
vc	0.896	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	681.45	J/mol×K	722.03	Joback Method
cpg	696.99	J/mol×K	752.31	Joback Method
cpg	711.72	J/mol×K	782.58	Joback Method
cpg	725.63	J/mol×K	812.86	Joback Method
cpg	738.75	J/mol×K	843.13	Joback Method
cpg	751.06	J/mol×K	873.41	Joback Method
cpg	762.59	J/mol×K	903.69	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320731&Units=SI

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