l-Norvaline, n-propoxycarbonyl-, isohexyl ester

Inchi: InChI=1S/C15H29NO4/c1-5-8-13(16-15(18)20-10-6-2)14(17)19-11-7-9-12(3)4/h12-13H,5

InchiKey: GKCHBDRPIZCEJQ-UHFFFAOYSA-N

Formula: C15H29NO4

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

Mol. weight [g/mol]: 287.40

Physical Properties

Property code	Value	Unit	Source
gf	-307.91	kJ/mol	Joback Method
hf	-799.62	kJ/mol	Joback Method
hfus	38.23	kJ/mol	Joback Method
hvap	72.96	kJ/mol	Joback Method
log10ws	-3.86		Crippen Method
logp	3.271		Crippen Method
mcvol	247.070	ml/mol	McGowan Method
pc	1553.67	kPa	Joback Method
rinpol	1706.00		NIST Webbook
rinpol	1706.00		NIST Webbook
tb	744.47	K	Joback Method
tc	928.33	K	Joback Method
tf	425.79	K	Joback Method
vc	0.947	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	738.37	J/mol×K	744.47	Joback Method
cpg	754.49	J/mol×K	775.11	Joback Method
cpg	769.73	J/mol×K	805.76	Joback Method
cpg	784.09	J/mol×K	836.40	Joback Method
cpg	797.58	J/mol×K	867.04	Joback Method
cpg	810.20	J/mol×K	897.69	Joback Method
cpg	821.97	J/mol×K	928.33	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=U320732&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