l-Norvaline, n-propoxycarbonyl-, isobutyl ester

Inchi: InChI=1S/C13H25NO4/c1-5-7-11(12(15)18-9-10(3)4)14-13(16)17-8-6-2/h10-11H,5-9H2,1
InchiKey: RPUMZARFNDQFRZ-UHFFFAOYSA-N
Formula: C13H25NO4
SMILES: CCCOC(=O)NC(CCC)C(=O)OCC(C)C
Mol. weight [g/mol]: 259.34

Physical Properties

Property code	Value	Unit	Source
gf	-324.75	kJ/mol	Joback Method
hf	-758.34	kJ/mol	Joback Method
hfus	33.05	kJ/mol	Joback Method
hvap	68.50	kJ/mol	Joback Method
log10ws	-3.03		Crippen Method
logp	2.490		Crippen Method
mcvol	218.890	ml/mol	McGowan Method
pc	1818.50	kPa	Joback Method
rinpol	1555.00		NIST Webbook
rinpol	1555.00		NIST Webbook
tb	698.71	K	Joback Method
tc	882.99	K	Joback Method
tf	403.25	K	Joback Method
vc	0.835	m3/kmol	Joback Method

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
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=U320729&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