

I-Norvaline, N-allyloxycarbonyl-, isobutyl ester

Inchi: InChI=1S/C13H23NO4/c1-5-7-11(12(15)18-9-10(3)4)14-13(16)17-8-6-2/h6,10-11H,2,5,7-
InchiKey: AMQSWXUBQPWHII-UHFFFAOYSA-N
Formula: C13H23NO4
SMILES: C=CCOC(=O)NC(CCC)C(=O)OCC(C)C
Mol. weight [g/mol]: 257.33

Physical Properties

Property code	Value	Unit	Source
gf	-236.91	kJ/mol	Joback Method
hf	-632.91	kJ/mol	Joback Method
hfus	31.77	kJ/mol	Joback Method
hvap	67.83	kJ/mol	Joback Method
log10ws	-2.88		Crippen Method
logp	2.267		Crippen Method
mcvol	214.590	ml/mol	McGowan Method
pc	1885.44	kPa	Joback Method
rinpola	1558.00		NIST Webbook
rinpola	1558.00		NIST Webbook
tb	695.39	K	Joback Method
tc	882.01	K	Joback Method
tf	401.49	K	Joback Method
vc	0.816	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	602.83	J/molxK	695.39	Joback Method
cpg	617.62	J/molxK	726.49	Joback Method
cpg	631.62	J/molxK	757.60	Joback Method
cpg	644.84	J/molxK	788.70	Joback Method
cpg	657.28	J/molxK	819.80	Joback Method
cpg	668.96	J/molxK	850.91	Joback Method
cpg	679.87	J/molxK	882.01	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320745&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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