

I-Norvaline, N-ethoxycarbonyl-, heptyl ester

Inchi:	InChI=1S/C15H29NO4/c1-4-7-8-9-10-12-20-14(17)13(11-5-2)16-15(18)19-6-3/h13H,4-12
InchiKey:	OMSGRJBLIMCAAT-UHFFFAOYSA-N
Formula:	C15H29NO4
SMILES:	CCCCCCCOC(=O)C(CCC)NC(=O)OCC
Mol. weight [g/mol]:	287.40

Physical Properties

Property code	Value	Unit	Source
gf	-305.47	kJ/mol	Joback Method
hf	-794.34	kJ/mol	Joback Method
hfus	41.76	kJ/mol	Joback Method
hvap	73.34	kJ/mol	Joback Method
log10ws	-4.11		Crippen Method
logp	3.415		Crippen Method
mvol	247.070	ml/mol	McGowan Method
pc	1543.92	kPa	Joback Method
rinpol	1752.00		NIST Webbook
rinpol	1752.00		NIST Webbook
tb	744.91	K	Joback Method
tc	926.88	K	Joback Method
tf	440.79	K	Joback Method
vc	0.953	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	737.86	J/molxK	744.91	Joback Method
cpg	753.81	J/molxK	775.24	Joback Method
cpg	768.89	J/molxK	805.57	Joback Method
cpg	783.13	J/molxK	835.90	Joback Method
cpg	796.51	J/molxK	866.22	Joback Method
cpg	809.06	J/molxK	896.55	Joback Method
cpg	820.77	J/molxK	926.88	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320704&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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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