

L-Norvaline, N-isobutoxycarbonyl-, heptadecyl ester

Inchi:	InChI=1S/C27H53NO4/c1-5-7-8-9-10-11-12-13-14-15-16-17-18-19-20-22-31-26(29)25(2
InchiKey:	OGWXZHRXYRVPPS-UHFFFAOYSA-N
Formula:	C27H53NO4
SMILES:	CCCCCCCCCCCCCCCCOC(=O)C(CCC)NC(=O)OCC(C)C
Mol. weight [g/mol]:	455.71

Physical Properties

Property code	Value	Unit	Source
gf	-206.87	kJ/mol	Joback Method
hf	-1047.30	kJ/mol	Joback Method
hfus	69.31	kJ/mol	Joback Method
hvap	99.67	kJ/mol	Joback Method
log10ws	-8.89		Crippen Method
logp	7.952		Crippen Method
mcvol	416.150	ml/mol	McGowan Method
pc	734.82	kPa	Joback Method
tb	1019.03	K	Joback Method
tc	1264.62	K	Joback Method
tf	561.03	K	Joback Method
vc	1.619	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1475.88	J/molxK	1019.03	Joback Method
cpg	1497.06	J/molxK	1059.96	Joback Method
cpg	1516.13	J/molxK	1100.89	Joback Method
cpg	1533.17	J/molxK	1141.82	Joback Method
cpg	1548.25	J/molxK	1182.75	Joback Method
cpg	1561.46	J/molxK	1223.68	Joback Method
cpg	1572.87	J/molxK	1264.62	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320725&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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