

L-Norvaline, N-allyloxycarbonyl-, octadecyl ester

Inchi:	InChI=1S/C27H51NO4/c1-4-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-24-31-26(29)2
InchiKey:	UFTVQVWZUHXYJP-UHFFFAOYSA-N
Formula:	C27H51NO4
SMILES:	C=CCOC(=O)NC(CCC)C(=O)OCCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]:	453.70

Physical Properties

Property code	Value	Unit	Source
gf	-116.59	kJ/mol	Joback Method
hf	-916.59	kJ/mol	Joback Method
hfus	71.56	kJ/mol	Joback Method
hvap	99.39	kJ/mol	Joback Method
log10ws	-8.98		Crippen Method
logp	7.872		Crippen Method
mcvol	411.850	ml/mol	McGowan Method
pc	748.56	kPa	Joback Method
tb	1016.15	K	Joback Method
tc	1260.55	K	Joback Method
tf	574.27	K	Joback Method
vc	1.605	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1445.08	J/molxK	1016.15	Joback Method
cpg	1465.94	J/molxK	1056.88	Joback Method
cpg	1484.84	J/molxK	1097.62	Joback Method
cpg	1501.84	J/molxK	1138.35	Joback Method
cpg	1517.04	J/molxK	1179.09	Joback Method
cpg	1530.51	J/molxK	1219.82	Joback Method
cpg	1542.36	J/molxK	1260.55	Joback Method

Sources

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=U320757&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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