

DL-Alanine, N-methyl-N-hexyloxycarbonyl-, heptadecyl ester

Inchi:	InChI=1S/C28H55NO4/c1-5-7-9-11-12-13-14-15-16-17-18-19-20-21-23-24-32-27(30)26(31)25
InchiKey:	IBDGTEUJBCCJNS-UHFFFAOYSA-N
Formula:	C28H55NO4
SMILES:	CCCCCCCCCCCCCCCCOC(=O)C(C)N(C)C(=O)OCCCCC
Mol. weight [g/mol]:	469.74

Physical Properties

Property code	Value	Unit	Source
gf	-174.62	kJ/mol	Joback Method
hf	-1048.60	kJ/mol	Joback Method
hfus	73.35	kJ/mol	Joback Method
hvap	97.89	kJ/mol	Joback Method
log10ws	-8.93		Crippen Method
logp	8.438		Crippen Method
mcvol	430.240	ml/mol	McGowan Method
pc	689.61	kPa	Joback Method
rinpol	3076.00		NIST Webbook
rinpol	3076.00		NIST Webbook
tb	1004.62	K	Joback Method
tc	1249.72	K	Joback Method
tf	567.11	K	Joback Method
vc	1.663	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1520.21	J/molxK	1004.62	Joback Method
cpg	1543.11	J/molxK	1045.47	Joback Method
cpg	1563.91	J/molxK	1086.32	Joback Method
cpg	1582.70	J/molxK	1127.17	Joback Method
cpg	1599.58	J/molxK	1168.02	Joback Method
cpg	1614.63	J/molxK	1208.87	Joback Method
cpg	1627.96	J/molxK	1249.72	Joback Method

Sources

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=U392646&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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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