

DL-Alanine, N-methyl-N-octyloxycarbonyl-, undecyl ester

Inchi: InChI=1S/C24H47NO4/c1-5-7-9-11-13-14-15-17-18-20-28-23(26)22(3)25(4)24(27)29-21-2
InchiKey: IUGFAMKQQSKNNF-UHFFFAOYSA-N
Formula: C24H47NO4
SMILES: CCCCCCCCCCOC(=O)C(C)N(C)C(=O)OCCCCCCCCC
Mol. weight [g/mol]: 413.63

Physical Properties

Property code	Value	Unit	Source
gf	-208.30	kJ/mol	Joback Method
hf	-966.04	kJ/mol	Joback Method
hfus	62.99	kJ/mol	Joback Method
hvap	88.98	kJ/mol	Joback Method
log10ws	-7.25		Crippen Method
logp	6.878		Crippen Method
mcvol	373.880	ml/mol	McGowan Method
pc	852.97	kPa	Joback Method
rinpol	2667.00		NIST Webbook
rinpol	2667.00		NIST Webbook
tb	913.10	K	Joback Method
tc	1119.88	K	Joback Method
tf	522.03	K	Joback Method
vc	1.440	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1262.61	J/mol×K	913.10	Joback Method
cpg	1282.96	J/mol×K	947.56	Joback Method
cpg	1301.84	J/mol×K	982.03	Joback Method
cpg	1319.30	J/mol×K	1016.49	Joback Method
cpg	1335.39	J/mol×K	1050.95	Joback Method
cpg	1350.15	J/mol×K	1085.42	Joback Method
cpg	1363.62	J/mol×K	1119.88	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U392653&Units=SI

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
rlnpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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