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

Inchi: InChI=1S/C26H51NO4/c1-5-7-9-11-13-15-17-18-20-22-30-25(28)24(3)27(4)26(29)31-23-

InchiKey: ZNDVEBVFUKVAOK-UHFFFAOYSA-N

Formula: C26H51NO4

SMILES: CCCCCCCCCCCOC(=O)C(C)N(C)C(=O)OCCCCCCCCCC

Mol. weight [g/mol]: 441.69

Physical Properties

Property code	Value	Unit	Source
gf	-191.46	kJ/mol	Joback Method
hf	-1007.32	kJ/mol	Joback Method
hfus	68.17	kJ/mol	Joback Method
hvap	93.44	kJ/mol	Joback Method
log10ws	-8.09		Crippen Method
logp	7.658		Crippen Method
mcvol	402.060	ml/mol	McGowan Method
pc	764.79	kPa	Joback Method
rinpol	2849.00		NIST Webbook
rinpol	2849.00		NIST Webbook
tb	958.86	K	Joback Method
tc	1182.25	K	Joback Method
tf	544.57	K	Joback Method
vc	1.552	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1390.62	J/mol×K	958.86	Joback Method
cpg	1412.14	J/mol×K	996.09	Joback Method
cpg	1431.93	J/mol×K	1033.32	Joback Method
cpg	1450.04	J/mol×K	1070.56	Joback Method
cpg	1466.53	J/mol×K	1107.79	Joback Method
cpg	1481.49	J/mol×K	1145.02	Joback Method
cpg	1494.96	J/mol×K	1182.25	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392681&Units=SI
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

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