DL-Alanine, N-methyl-N-(2-ethylhexyloxycarbonyl)-, octadecyl ester

Inchi: InChI=1S/C31H61NO4/c1-6-9-11-12-13-14-15-16-17-18-19-20-21-22-23-24-26-35-30(33
InchiKey: CESNFJYVGUNCQM-UHFFFAOYSA-N
Formula: C31H61NO4
SMILES: CCCCCCCCCCCCCCCCCCOC(=O)C(C)N(C)C(=O)OCC(CC)CCCC
Mol. weight [g/mol]: 511.82

Physical Properties

Property code	Value	Unit	Source
gf	-151.80	kJ/mol	Joback Method
hf	-1115.80	kJ/mol	Joback Method
hfus	77.59	kJ/mol	Joback Method
hvap	104.18	kJ/mol	Joback Method
log10ws	-9.94		Crippen Method
logp	9.464		Crippen Method
mcvol	472.510	ml/mol	McGowan Method
pc	598.38	kPa	Joback Method
rinpol	3282.00		NIST Webbook
rinpol	3282.00		NIST Webbook
tb	1072.82	K	Joback Method
tc	1357.65	K	Joback Method
tf	585.92	K	Joback Method
vc	1.825	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1716.91	J/mol×K	1072.82	Joback Method
cpg	1741.83	J/mol×K	1120.29	Joback Method
cpg	1763.93	J/mol×K	1167.76	Joback Method
cpg	1783.38	J/mol×K	1215.23	Joback Method
cpg	1800.34	J/mol×K	1262.71	Joback Method
cpg	1814.99	J/mol×K	1310.18	Joback Method
cpg	1827.50	J/mol×K	1357.65	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=U392669&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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
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

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