DL-3-Aminobutanoic acid, N-(2-ethylhexyl)oxycarbonyl-, hexadecyl ester

Inchi: InChI=1S/C29H57NO4/c1-5-8-10-11-12-13-14-15-16-17-18-19-20-21-23-33-28(31)24-26

InchiKey: NVSIAENGIDMRNK-UHFFFAOYSA-N

Formula: C29H57NO4

SMILES: CCCCCCCCCCCCCCCCOC(=O)CC(C)NC(=O)OCC(CC)CCCC

Mol. weight [g/mol]: 483.77

Physical Properties

Property code	Value	Unit	Source
gf	-190.03	kJ/mol	Joback Method
hf	-1088.58	kJ/mol	Joback Method
hfus	74.49	kJ/mol	Joback Method
hvap	104.12	kJ/mol	Joback Method
log10ws	-9.72		Crippen Method
logp	8.732		Crippen Method
mcvol	444.330	ml/mol	McGowan Method
pc	663.92	kPa	Joback Method
rinpol	3286.00		NIST Webbook
rinpol	3286.00		NIST Webbook
tb	1064.79	K	Joback Method
tc	1336.93	K	Joback Method
tf	583.57	K	Joback Method
vc	1.730	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1605.29	J/mol×K	1064.79	Joback Method
cpg	1627.74	J/mol×K	1110.15	Joback Method
cpg	1647.60	J/mol×K	1155.50	Joback Method
cpg	1664.98	J/mol×K	1200.86	Joback Method
cpg	1680.01	J/mol×K	1246.22	Joback Method
cpg	1692.81	J/mol×K	1291.57	Joback Method
cpg	1703.49	J/mol×K	1336.93	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392828&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