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

Inchi: InChI=1S/C17H33NO4/c1-5-8-10-15(7-3)13-22-17(20)18-14(4)12-16(19)21-11-9-6-2/h14

InchiKey: QTFIGKRLCNEQPI-UHFFFAOYSA-N

Formula: C17H33NO4

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

Mol. weight [g/mol]: 315.45

Physical Properties

Property code	Value	Unit	Source
gf	-291.07	kJ/mol	Joback Method
hf	-840.90	kJ/mol	Joback Method
hfus	43.41	kJ/mol	Joback Method
hvap	77.41	kJ/mol	Joback Method
log10ws	-4.70		Crippen Method
logp	4.051		Crippen Method
mcvol	275.250	ml/mol	McGowan Method
pc	1342.74	kPa	Joback Method
rinpol	2133.00		NIST Webbook
rinpol	2133.00		NIST Webbook
tb	790.23	K	Joback Method
tc	975.91	K	Joback Method
tf	448.33	K	Joback Method
vc	1.058	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	854.25	J/mol×K	790.23	Joback Method
cpg	871.09	J/mol×K	821.18	Joback Method
cpg	886.93	J/mol×K	852.12	Joback Method
cpg	901.80	J/mol×K	883.07	Joback Method
cpg	915.70	J/mol×K	914.02	Joback Method
cpg	928.66	J/mol×K	944.97	Joback Method
cpg	940.67	J/mol×K	975.91	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=U392817&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume