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

Inchi: InChI=1S/C17H33NO4/c1-6-8-9-15(7-2)12-22-17(20)18-14(5)10-16(19)21-11-13(3)4/h13

InchiKey: YDRRRHKNXVOBPT-UHFFFAOYSA-N

Formula: C17H33NO4

SMILES: CCCCC(CC)COC(=O)NC(C)CC(=O)OCC(C)C

Mol. weight [g/mol]: 315.45

Physical Properties

Property code	Value	Unit	Source
gf	-293.51	kJ/mol	Joback Method
hf	-846.18	kJ/mol	Joback Method
hfus	39.89	kJ/mol	Joback Method
hvap	77.02	kJ/mol	Joback Method
log10ws	-4.46		Crippen Method
logp	3.907		Crippen Method
mcvol	275.250	ml/mol	McGowan Method
pc	1350.65	kPa	Joback Method
rinpol	2095.00		NIST Webbook
rinpol	2095.00		NIST Webbook
tb	789.79	K	Joback Method
tc	976.92	K	Joback Method
tf	433.33	K	Joback Method
vc	1.052	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	854.76	J/mol×K	789.79	Joback Method
cpg	871.73	J/mol×K	820.98	Joback Method
cpg	887.68	J/mol×K	852.17	Joback Method
cpg	902.64	J/mol×K	883.35	Joback Method
cpg	916.60	J/mol×K	914.54	Joback Method
cpg	929.59	J/mol×K	945.73	Joback Method
cpg	941.62	J/mol×K	976.92	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392816&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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