DL-3-Aminobutanoic acid, N-hexyloxycarbonyl-, hexyl ester

Inchi: InChI=1S/C17H33NO4/c1-4-6-8-10-12-21-16(19)14-15(3)18-17(20)22-13-11-9-7-5-2/h15

InchiKey: BZDDEXPMKHDDOQ-UHFFFAOYSA-N

Formula: C17H33NO4

SMILES: CCCCCCOC(=O)CC(C)NC(=O)OCCCCCC

Mol. weight [g/mol]: 315.45

Physical Properties

Property code	Value	Unit	Source
gf	-288.63	kJ/mol	Joback Method
hf	-835.62	kJ/mol	Joback Method
hfus	46.94	kJ/mol	Joback Method
hvap	77.80	kJ/mol	Joback Method
log10ws	-4.94		Crippen Method
logp	4.195		Crippen Method
mcvol	275.250	ml/mol	McGowan Method
pc	1334.91	kPa	Joback Method
rinpol	2133.00		NIST Webbook
rinpol	2133.00		NIST Webbook
tb	790.67	K	Joback Method
tc	975.04	K	Joback Method
tf	463.33	K	Joback Method
vc	1.065	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	853.75	J/mol×K	790.67	Joback Method
cpg	870.46	J/mol×K	821.40	Joback Method
cpg	886.20	J/mol×K	852.13	Joback Method
cpg	900.99	J/mol×K	882.86	Joback Method
cpg	914.84	J/mol×K	913.59	Joback Method
cpg	927.76	J/mol×K	944.31	Joback Method
cpg	939.76	J/mol×K	975.04	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392809&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