1-Aminocyclopentanecarboxylic acid, N-(hexyloxycarbonyl)-, propyl ester

Inchi: InChI=1S/C16H29NO4/c1-3-5-6-9-13-21-15(19)17-16(10-7-8-11-16)14(18)20-12-4-2/h3-1

InchiKey: OBAJDUYHDKRBAG-UHFFFAOYSA-N

Formula: C16H29NO4

SMILES: CCCCCCOC(=O)NC1(C(=O)OCCC)CCCC1

Mol. weight [g/mol]: 299.41

Physical Properties

Property code	Value	Unit	Source
gf	-263.55	kJ/mol	Joback Method
hf	-733.98	kJ/mol	Joback Method
hfus	35.51	kJ/mol	Joback Method
hvap	75.06	kJ/mol	Joback Method
log10ws	-4.42		Crippen Method
logp	3.559		Crippen Method
mcvol	250.300	ml/mol	McGowan Method
pc	1701.90	kPa	Joback Method
rinpol	2015.00		NIST Webbook
rinpol	2015.00		NIST Webbook
tb	783.75	K	Joback Method
tc	982.67	K	Joback Method
tf	501.86	K	Joback Method
vc	0.954	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	781.83	J/mol×K	783.75	Joback Method
cpg	799.56	J/mol×K	816.90	Joback Method
cpg	816.60	J/mol×K	850.06	Joback Method
cpg	833.03	J/mol×K	883.21	Joback Method
cpg	848.94	J/mol×K	916.37	Joback Method
cpg	864.41	J/mol×K	949.52	Joback Method
cpg	879.54	J/mol×K	982.67	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392558&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