1-Aminocyclopentanecarboxylic acid, N-(isobutoxycarbonyl)-, pentyl ester

Inchi: InChI=1S/C16H29NO4/c1-4-5-8-11-20-14(18)16(9-6-7-10-16)17-15(19)21-12-13(2)3/h13

InchiKey: VJNGQUXZWOPSEI-UHFFFAOYSA-N

Formula: C16H29NO4

SMILES: CCCCCOC(=O)C1(NC(=O)OCC(C)C)CCCC1

Mol. weight [g/mol]: 299.41

Physical Properties

Property code	Value	Unit	Source
gf	-265.99	kJ/mol	Joback Method
hf	-739.26	kJ/mol	Joback Method
hfus	31.98	kJ/mol	Joback Method
hvap	74.68	kJ/mol	Joback Method
log10ws	-4.18		Crippen Method
logp	3.415		Crippen Method
mcvol	250.300	ml/mol	McGowan Method
pc	1713.19	kPa	Joback Method
rinpol	1987.00		NIST Webbook
rinpol	1987.00		NIST Webbook
tb	783.31	K	Joback Method
tc	984.69	K	Joback Method
tf	486.86	K	Joback Method
vc	0.948	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	782.34	J/mol×K	783.31	Joback Method
cpg	800.29	J/mol×K	816.87	Joback Method
cpg	817.52	J/mol×K	850.44	Joback Method
cpg	834.12	J/mol×K	884.00	Joback Method
cpg	850.17	J/mol×K	917.56	Joback Method
cpg	865.78	J/mol×K	951.13	Joback Method
cpg	881.02	J/mol×K	984.69	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392503&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