1-Aminocyclopentanecarboxylic acid, N-(2-methoxyethoxycarbonyl)-, isobutyl ester

Inchi: InChI=1S/C14H25NO5/c1-11(2)10-20-12(16)14(6-4-5-7-14)15-13(17)19-9-8-18-3/h11H,4

InchiKey: OSJLWJFVEUHYSJ-UHFFFAOYSA-N

Formula: C14H25NO5

SMILES: COCCOC(=O)NC1(C(=O)OCC(C)C)CCCC1

Mol. weight [g/mol]: 287.35

Physical Properties

Property code	Value	Unit	Source
gf	-387.83	kJ/mol	Joback Method
hf	-830.20	kJ/mol	Joback Method
hfus	27.99	kJ/mol	Joback Method
hvap	72.63	kJ/mol	Joback Method
log10ws	-2.43		Crippen Method
logp	1.871		Crippen Method
mcvol	227.990	ml/mol	McGowan Method
pc	1991.21	kPa	Joback Method
rinpol	1908.00		NIST Webbook
rinpol	1908.00		NIST Webbook
tb	759.97	K	Joback Method
tc	963.31	K	Joback Method
tf	486.55	K	Joback Method
vc	0.854	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	696.72	J/mol×K	759.97	Joback Method
cpg	713.57	J/mol×K	793.86	Joback Method
cpg	729.70	J/mol×K	827.75	Joback Method
cpg	745.18	J/mol×K	861.64	Joback Method
cpg	760.08	J/mol×K	895.53	Joback Method
cpg	774.48	J/mol×K	929.42	Joback Method
cpg	788.46	J/mol×K	963.31	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=U392546&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