1-Aminocyclopentanecarboxylic acid, N-(propoxycarbonyl)-, isobutyl ester

Inchi: InChI=1S/C14H25NO4/c1-4-9-18-13(17)15-14(7-5-6-8-14)12(16)19-10-11(2)3/h11H,4-10

InchiKey: JJQZRPZQZFBGKL-UHFFFAOYSA-N

Formula: C14H25NO4

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

Mol. weight [g/mol]: 271.35

Physical Properties

Property code	Value	Unit	Source
gf	-282.83	kJ/mol	Joback Method
hf	-697.98	kJ/mol	Joback Method
hfus	26.80	kJ/mol	Joback Method
hvap	70.22	kJ/mol	Joback Method
log10ws	-3.34		Crippen Method
logp	2.635		Crippen Method
mcvol	222.120	ml/mol	McGowan Method
pc	2021.76	kPa	Joback Method
rinpol	1793.00		NIST Webbook
rinpol	1793.00		NIST Webbook
tb	737.55	K	Joback Method
tc	941.93	K	Joback Method
tf	464.32	K	Joback Method
vc	0.836	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	667.85	J/mol×K	737.55	Joback Method
cpg	684.95	J/mol×K	771.61	Joback Method
cpg	701.30	J/mol×K	805.68	Joback Method
cpg	717.00	J/mol×K	839.74	Joback Method
cpg	732.13	J/mol×K	873.80	Joback Method
cpg	746.77	J/mol×K	907.86	Joback Method
cpg	761.03	J/mol×K	941.93	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392500&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