Cyclopentanecarboxylic acid, 3-carbamoyl-, cis , benzyl ester

Inchi: InChI=1S/C14H17NO3/c15-13(16)11-6-7-12(8-11)14(17)18-9-10-4-2-1-3-5-10/h1-5,11-12

InchiKey: WJYZBHHXSBEBJY-NEPJUHHUSA-N

Formula: C14H17NO3

SMILES: NC(=O)C1CCC(C(=O)OCc2ccccc2)C1

Mol. weight [g/mol]: 247.29

Physical Properties

Property code	Value	Unit	Source
gf	-88.14	kJ/mol	Joback Method
hf	-379.21	kJ/mol	Joback Method
hfus	30.65	kJ/mol	Joback Method
hvap	75.52	kJ/mol	Joback Method
log10ws	-2.76		Crippen Method
logp	1.631		Crippen Method
mcvol	192.490	ml/mol	McGowan Method
pc	2718.33	kPa	Joback Method
tb	759.70	K	Joback Method
tc	998.64	K	Joback Method
tf	485.97	K	Joback Method
vc	0.711	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	570.52	J/mol×K	759.70	Joback Method
cpg	586.17	J/mol×K	799.52	Joback Method
cpg	600.47	J/mol×K	839.35	Joback Method
cpg	613.48	J/mol×K	879.17	Joback Method
cpg	625.24	J/mol×K	919.00	Joback Method
cpg	635.81	J/mol×K	958.82	Joback Method
cpg	645.24	J/mol×K	998.64	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=B6010451&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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