Cyclopentanecarboxylic acid, 4-cyanophenyl ester

Inchi: InChI=1S/C13H13NO2/c14-9-10-5-7-12(8-6-10)16-13(15)11-3-1-2-4-11/h5-8,11H,1-4H2
InchiKey: ROZSAQJIZMVUKD-UHFFFAOYSA-N
Formula: C13H13NO2
SMILES: N#Cc1ccc(OC(=O)C2CCCC2)cc1
Mol. weight [g/mol]: 215.25

Physical Properties

Property code	Value	Unit	Source
gf	97.17	kJ/mol	Joback Method
hf	-106.03	kJ/mol	Joback Method
hfus	21.31	kJ/mol	Joback Method
hvap	67.36	kJ/mol	Joback Method
log10ws	-3.47		Crippen Method
logp	2.654		Crippen Method
mcvol	168.230	ml/mol	McGowan Method
pc	2632.55	kPa	Joback Method
rinpol	1779.00		NIST Webbook
rinpol	1779.00		NIST Webbook
tb	722.15	K	Joback Method
tc	966.93	K	Joback Method
tf	423.26	K	Joback Method
vc	0.646	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	460.05	J/mol×K	722.15	Joback Method
cpg	474.38	J/mol×K	762.95	Joback Method
cpg	487.52	J/mol×K	803.74	Joback Method
cpg	499.54	J/mol×K	844.54	Joback Method
cpg	510.46	J/mol×K	885.34	Joback Method
cpg	520.35	J/mol×K	926.14	Joback Method
cpg	529.23	J/mol×K	966.93	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=U307578&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