Cyclohexanecarboxylic acid, 4-cyanophenyl ester

Inchi: InChI=1S/C14H15NO2/c15-10-11-6-8-13(9-7-11)17-14(16)12-4-2-1-3-5-12/h6-9,12H,1-5
InchiKey: UHVXYUDWPRIRGD-UHFFFAOYSA-N
Formula: C14H15NO2
SMILES: N#Cc1ccc(OC(=O)C2CCCCC2)cc1
Mol. weight [g/mol]: 229.27

Physical Properties

Property code	Value	Unit	Source
gf	93.49	kJ/mol	Joback Method
hf	-132.83	kJ/mol	Joback Method
hfus	21.80	kJ/mol	Joback Method
hvap	69.76	kJ/mol	Joback Method
log10ws	-3.88		Crippen Method
logp	3.044		Crippen Method
mcvol	182.320	ml/mol	McGowan Method
pc	2450.74	kPa	Joback Method
rinpol	1896.00		NIST Webbook
rinpol	1896.00		NIST Webbook
tb	749.30	K	Joback Method
tc	996.36	K	Joback Method
tf	431.01	K	Joback Method
vc	0.695	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	515.61	J/mol×K	749.30	Joback Method
cpg	530.96	J/mol×K	790.48	Joback Method
cpg	544.97	J/mol×K	831.65	Joback Method
cpg	557.67	J/mol×K	872.83	Joback Method
cpg	569.11	J/mol×K	914.01	Joback Method
cpg	579.33	J/mol×K	955.18	Joback Method
cpg	588.37	J/mol×K	996.36	Joback Method

Sources

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=U307706&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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