4-Chlorobenzoic acid, 4-cyanophenyl ester

Inchi: InChI=1S/C14H8ClNO2/c15-12-5-3-11(4-6-12)14(17)18-13-7-1-10(9-16)2-8-13/h1-8H
InchiKey: PGPBOUBXPMLQLM-UHFFFAOYSA-N
Formula: C14H8ClNO2
SMILES: N#Cc1ccc(OC(=O)c2ccc(Cl)cc2)cc1
Mol. weight [g/mol]: 257.67

Physical Properties

Property code	Value	Unit	Source
gf	159.89	kJ/mol	Joback Method
hf	22.17	kJ/mol	Joback Method
hfus	27.81	kJ/mol	Joback Method
hvap	76.65	kJ/mol	Joback Method
log10ws	-4.60		Crippen Method
logp	3.431		Crippen Method
mcvol	181.660	ml/mol	McGowan Method
pc	2640.67	kPa	Joback Method
rinpol	2131.00		NIST Webbook
rinpol	2131.00		NIST Webbook
tb	798.84	K	Joback Method
tc	1055.44	K	Joback Method
tf	492.49	K	Joback Method
vc	0.703	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	451.68	J/mol×K	798.84	Joback Method
cpg	461.84	J/mol×K	841.61	Joback Method
cpg	470.96	J/mol×K	884.37	Joback Method
cpg	479.08	J/mol×K	927.14	Joback Method
cpg	486.24	J/mol×K	969.91	Joback Method
cpg	492.50	J/mol×K	1012.67	Joback Method
cpg	497.90	J/mol×K	1055.44	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=U307760&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