

4-Cyanobenzoic acid, 2-chlorophenyl ester

Inchi:	InChI=1S/C14H8ClNO2/c15-12-3-1-2-4-13(12)18-14(17)11-7-5-10(9-16)6-8-11/h1-8H
InchiKey:	WNVUMPBLXYWKLI-UHFFFAOYSA-N
Formula:	C14H8ClNO2
SMILES:	N#Cc1ccc(C(=O)Oc2ccccc2Cl)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
rinqol	1962.20		NIST Webbook
tb	798.84	K	Joback Method
tc	1055.44	K	Joback Method
tf	492.49	K	Joback Method
vc	0.703	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	451.68	J/molxK	798.84	Joback Method
cpg	461.84	J/molxK	841.61	Joback Method
cpg	470.96	J/molxK	884.37	Joback Method
cpg	479.08	J/molxK	927.14	Joback Method
cpg	486.24	J/molxK	969.91	Joback Method
cpg	492.50	J/molxK	1012.67	Joback Method
cpg	497.90	J/molxK	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=U292658&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
mccvol:	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

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