

4-Chloro-2-cyclohexylphenol

Other names:	Phenol, 4-chloro-2-cyclohexyl- 2-Cyclohexyl-4-chlorophenol
Inchi:	InChI=1S/C12H15ClO/c13-10-6-7-12(14)11(8-10)9-4-2-1-3-5-9/h6-9,14H,1-5H2
InchiKey:	XRUHXAQEOJDPEG-UHFFFAOYSA-N
Formula:	C12H15ClO
SMILES:	Oc1ccc(Cl)cc1C1CCCCC1
Mol. weight [g/mol]:	210.70
CAS:	13081-17-9

Physical Properties

Property code	Value	Unit	Source
gf	10.84	kJ/mol	Joback Method
hf	-204.68	kJ/mol	Joback Method
hfus	22.30	kJ/mol	Joback Method
hvap	63.07	kJ/mol	Joback Method
log10ws	-4.04		Crippen Method
logp	4.093		Crippen Method
mvol	163.430	ml/mol	McGowan Method
pc	3314.37	kPa	Joback Method
tb	643.22	K	Joback Method
tc	898.99	K	Joback Method
tf	412.96	K	Joback Method
vc	0.547	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	421.91	J/mol×K	643.22	Joback Method
cpg	439.02	J/mol×K	685.85	Joback Method
cpg	454.79	J/mol×K	728.48	Joback Method
cpg	469.37	J/mol×K	771.11	Joback Method
cpg	482.87	J/mol×K	813.73	Joback Method
cpg	495.44	J/mol×K	856.36	Joback Method
cpg	507.20	J/mol×K	898.99	Joback Method

dvisc	0.0010666	Paxs	412.96	Joback Method
dvisc	0.0004463	Paxs	451.34	Joback Method
dvisc	0.0002141	Paxs	489.71	Joback Method
dvisc	0.0001143	Paxs	528.09	Joback Method
dvisc	0.0000664	Paxs	566.47	Joback Method
dvisc	0.0000413	Paxs	604.84	Joback Method
dvisc	0.0000272	Paxs	643.22	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13081179&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
dvisc:	Dynamic viscosity
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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