

Phenol, 2-chloro-4-cyclohexyl-

Other names:	2-Chloro-4-cyclohexylphenol
Inchi:	InChI=1S/C12H15ClO/c13-11-8-10(6-7-12(11)14)9-4-2-1-3-5-9/h6-9,14H,1-5H2
InchiKey:	VVMQAIJCWNJCMK-UHFFFAOYSA-N
Formula:	C12H15ClO
SMILES:	Oc1ccc(C2CCCCC2)cc1Cl
Mol. weight [g/mol]:	210.70
CAS:	3964-61-2

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
mcvol	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	m3/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	Pa×s	412.96	Joback Method

dvisc	0.0004463	Pa×s	451.34	Joback Method
dvisc	0.0002141	Pa×s	489.71	Joback Method
dvisc	0.0001143	Pa×s	528.09	Joback Method
dvisc	0.0000664	Pa×s	566.47	Joback Method
dvisc	0.0000413	Pa×s	604.84	Joback Method
dvisc	0.0000272	Pa×s	643.22	Joback Method

Sources

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=C3964612&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
mccvol:	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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