

# 6-Chloro-2,4-diisopropyl phenol

<b>Inchi:</b>	InChI=1S/C12H17ClO/c1-7(2)9-5-10(8(3)4)12(14)11(13)6-9/h5-8,14H,1-4H3
<b>InchiKey:</b>	SVBPZUZWTSMLKY-UHFFFAOYSA-N
<b>Formula:</b>	C12H17ClO
<b>SMILES:</b>	CC(C)c1cc(Cl)c(O)c(C(C)C)c1
<b>Mol. weight [g/mol]:</b>	212.72
<b>CAS:</b>	102127-39-9

## Physical Properties

Property code	Value	Unit	Source
gf	-28.12	kJ/mol	Joback Method
hf	-281.03	kJ/mol	Joback Method
hfus	23.03	kJ/mol	Joback Method
hvap	62.53	kJ/mol	Joback Method
log10ws	-4.07		Crippen Method
logp	4.292		Crippen Method
mcvol	174.290	ml/mol	McGowan Method
pc	2654.29	kPa	Joback Method
tb	627.77	K	Joback Method
tc	853.57	K	Joback Method
tf	388.10	K	Joback Method
vc	0.603	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	432.39	J/molxK	627.77	Joback Method
cpg	496.61	J/molxK	815.93	Joback Method
cpg	485.23	J/molxK	778.30	Joback Method
cpg	473.19	J/molxK	740.67	Joback Method
cpg	460.42	J/molxK	703.04	Joback Method
cpg	446.85	J/molxK	665.40	Joback Method
cpg	507.43	J/molxK	853.57	Joback Method
dvisc	0.0000238	Paxs	627.77	Joback Method
dvisc	0.0000372	Paxs	587.83	Joback Method

dvisc	0.0000620	Paxs	547.88	Joback Method
dvisc	0.0001122	Paxs	507.94	Joback Method
dvisc	0.0002247	Paxs	467.99	Joback Method
dvisc	0.0005120	Paxs	428.05	Joback Method
dvisc	0.0013825	Paxs	388.10	Joback Method

## Sources

<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C102127399&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C102127399&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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