

# 1-Phenylcyclohexane-1,2-diol cis-

<b>Inchi:</b>	InChI=1S/C12H16O2/c13-11-8-4-5-9-12(11,14)10-6-2-1-3-7-10/h1-3,6-7,11,13-14H,4-5,8
<b>InchiKey:</b>	QHNHEYDAIICUDL-RYUDHWPBXSA-N
<b>Formula:</b>	C12H16O2
<b>SMILES:</b>	OC1CCCCC1(O)c1ccccc1
<b>Mol. weight [g/mol]:</b>	192.25
<b>CAS:</b>	4912-59-8

## Physical Properties

Property code	Value	Unit	Source
chs	-6540.00	kJ/mol	NIST Webbook
chs	-6532.90 ± 0.40	kJ/mol	NIST Webbook
gf	-99.82	kJ/mol	Joback Method
hf	-309.72	kJ/mol	Joback Method
hfus	15.66	kJ/mol	Joback Method
hvap	76.91	kJ/mol	Joback Method
log10ws	-2.65		Crippen Method
logp	1.809		Crippen Method
mcvol	157.060	ml/mol	McGowan Method
pc	3727.11	kPa	Joback Method
tb	700.12	K	Joback Method
tc	912.50	K	Joback Method
tf	400.10	K	Joback Method
vc	0.568	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	452.96	J/mol×K	700.12	Joback Method
cpg	466.74	J/mol×K	735.52	Joback Method
cpg	479.83	J/mol×K	770.91	Joback Method
cpg	492.35	J/mol×K	806.31	Joback Method
cpg	504.44	J/mol×K	841.71	Joback Method
cpg	516.21	J/mol×K	877.10	Joback Method
cpg	527.78	J/mol×K	912.50	Joback Method

# Sources

<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=C4912598&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C4912598&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.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>

# Legend

<b>chs:</b>	Standard solid enthalpy of combustion
<b>cpg:</b>	Ideal gas heat capacity
<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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