

# 1,4-Cyclohexanedicarboxylic acid

<b>Other names:</b>	1,4-Cyclohexanedicarboxylic acid,c&t 1,4-Dicarboxycyclohexane Hexahydroterephthalic acid Terephthalic acid, hexahydro- cyclohexane-1,4-dicarboxylic acid
<b>Inchi:</b>	InChI=1S/C8H12O4/c9-7(10)5-1-2-6(4-3-5)8(11)12/h5-6H,1-4H2,(H,9,10)(H,11,12)
<b>InchiKey:</b>	PXGZQGDTEZPERC-UHFFFAOYSA-N
<b>Formula:</b>	C8H12O4
<b>SMILES:</b>	O=C(O)C1CCC(C(=O)O)CC1
<b>Mol. weight [g/mol]:</b>	172.18
<b>CAS:</b>	1076-97-7

## Physical Properties

Property code	Value	Unit	Source
gf	-498.26	kJ/mol	Joback Method
hf	-704.09	kJ/mol	Joback Method
hfus	20.76	kJ/mol	Joback Method
hvap	80.37	kJ/mol	Joback Method
log10ws	-0.78		Crippen Method
logp	0.962		Crippen Method
mcvol	127.600	ml/mol	McGowan Method
pc	4420.84	kPa	Joback Method
tb	689.42	K	Joback Method
tc	884.77	K	Joback Method
tf	404.56	K	Joback Method
vc	0.466	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	365.11	J/molxK	689.42	Joback Method
cpg	410.91	J/molxK	852.21	Joback Method
cpg	403.04	J/molxK	819.65	Joback Method
cpg	394.53	J/molxK	787.09	Joback Method

cpg	385.38	J/molxK	754.54	Joback Method
cpg	375.58	J/molxK	721.98	Joback Method
cpg	418.18	J/molxK	884.77	Joback Method
dvisc	0.0000278	Paxs	689.42	Joback Method
dvisc	0.0000469	Paxs	641.94	Joback Method
dvisc	0.0000859	Paxs	594.47	Joback Method
dvisc	0.0001750	Paxs	546.99	Joback Method
dvisc	0.0004080	Paxs	499.51	Joback Method
dvisc	0.0011364	Paxs	452.04	Joback Method
dvisc	0.0040256	Paxs	404.56	Joback Method

## Sources

<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>
<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=C1076977&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C1076977&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>

## 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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