

# Cyclohexane-1,1-dicarboxylic acid

<b>Inchi:</b>	InChI=1S/C8H12O4/c9-6(10)8(7(11)12)4-2-1-3-5-8/h1-5H2,(H,9,10)(H,11,12)
<b>InchiKey:</b>	QYQADNCHXSEGJT-UHFFFAOYSA-N
<b>Formula:</b>	C8H12O4
<b>SMILES:</b>	O=C(O)C1(C(=O)O)CCCCC1
<b>Mol. weight [g/mol]:</b>	172.18
<b>CAS:</b>	1127-08-8

## Physical Properties

Property code	Value	Unit	Source
chs	-3893.60 ± 0.30	kJ/mol	NIST Webbook
gf	-496.04	kJ/mol	Joback Method
hf	-668.51	kJ/mol	Joback Method
hfus	13.39	kJ/mol	Joback Method
hvap	79.53	kJ/mol	Joback Method
log10ws	-1.02		Crippen Method
logp	1.106		Crippen Method
mvol	127.600	ml/mol	McGowan Method
pc	4917.69	kPa	Joback Method
tb	694.33	K	Joback Method
tc	895.74	K	Joback Method
tf	432.70	K	Joback Method
vc	0.465	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	357.60	J/mol×K	694.33	Joback Method
cpg	367.51	J/mol×K	727.90	Joback Method
cpg	376.99	J/mol×K	761.47	Joback Method
cpg	386.13	J/mol×K	795.03	Joback Method
cpg	395.03	J/mol×K	828.60	Joback Method
cpg	403.76	J/mol×K	862.17	Joback Method
cpg	412.42	J/mol×K	895.74	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C1127088&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C1127088&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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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