

# 1,1-Cyclohexane diacetic acid

<b>Inchi:</b>	InChI=1S/C10H16O4/c11-8(12)6-10(7-9(13)14)4-2-1-3-5-10/h1-7H2,(H,11,12)(H,13,14)
<b>InchiKey:</b>	YQPCHPBGAALCRT-UHFFFAOYSA-N
<b>Formula:</b>	C10H16O4
<b>SMILES:</b>	O=C(O)CC1(CC(=O)O)CCCCC1
<b>Mol. weight [g/mol]:</b>	200.23
<b>CAS:</b>	9355-11-7

## Physical Properties

Property code	Value	Unit	Source
gf	-479.20	kJ/mol	Joback Method
hf	-709.79	kJ/mol	Joback Method
hfus	18.57	kJ/mol	Joback Method
hvap	83.98	kJ/mol	Joback Method
log10ws	-1.86		Crippen Method
logp	1.886		Crippen Method
mcvol	155.780	ml/mol	McGowan Method
pc	3819.82	kPa	Joback Method
tb	740.09	K	Joback Method
tc	937.83	K	Joback Method
tf	455.24	K	Joback Method
vc	0.577	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	459.85	J/molxK	740.09	Joback Method
cpg	471.21	J/molxK	773.05	Joback Method
cpg	482.17	J/molxK	806.00	Joback Method
cpg	492.79	J/molxK	838.96	Joback Method
cpg	503.19	J/molxK	871.92	Joback Method
cpg	513.43	J/molxK	904.87	Joback Method
cpg	523.63	J/molxK	937.83	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=C9355117&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C9355117&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>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>h vap:</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>m cvol:</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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