

# cis-1,2,3,6-Tetrahydrophthalic anhydride

<b>Other names:</b>	Tetrahydrophthalic anhydride cis-4-Cyclohexene-1,2-dicarboxylic anhydride 1,3-Isobenzofurandione, 3a,4,7,7a-tetrahydro-, cis- cis-3a,4,7,7a-Tetrahydro-1,3-isobenzofurandione 3a,4,7,7a-Tetrahydro-2-benzofuran-1,3-dione, (Z)- 1,3-Isobenzofurandione, 3a,4,7,7a-tetrahydro-, (3aR,7aS)-rel-
<b>Inchi:</b>	InChI=1S/C8H8O3/c9-7-5-3-1-2-4-6(5)8(10)11-7/h1-2,5-6H,3-4H2/t5-,6+
<b>InchiKey:</b>	KMOUUVZVZFCRAM-OLQVQODUSA-N
<b>Formula:</b>	C8H8O3
<b>SMILES:</b>	O=C1OC(=O)C2CC=CCC12
<b>Mol. weight [g/mol]:</b>	152.15
<b>CAS:</b>	935-79-5

## Physical Properties

Property code	Value	Unit	Source
chs	-3519.00 ± 2.00	kJ/mol	NIST Webbook
gf	-199.66	kJ/mol	Joback Method
hf	-430.95	kJ/mol	Joback Method
hfs	-772.00 ± 2.00	kJ/mol	NIST Webbook
hfus	14.67	kJ/mol	Joback Method
hvap	47.04	kJ/mol	Joback Method
log10ws	-0.97		Crippen Method
logp	0.652		Crippen Method
mcvol	106.570	ml/mol	McGowan Method
pc	4140.93	kPa	Joback Method
tb	570.48	K	Joback Method
tc	825.93	K	Joback Method
tf	369.01	K	Joback Method
tt	371.60 ± 1.50	K	NIST Webbook
vc	0.395	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	340.45	J/mol×K	783.36	Joback Method
cpg	272.11	J/mol×K	570.48	Joback Method
cpg	287.75	J/mol×K	613.06	Joback Method
cpg	302.42	J/mol×K	655.63	Joback Method
cpg	316.11	J/mol×K	698.21	Joback Method
cpg	328.79	J/mol×K	740.78	Joback Method
cpg	351.08	J/mol×K	825.93	Joback Method
hsubt	53.10 ± 0.20	kJ/mol	325.00	NIST Webbook
hvapt	53.10 ± 0.10	kJ/mol	425.00	NIST Webbook

## 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=C935795&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C935795&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>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>hfs:</b>	Solid phase enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hsubt:</b>	Enthalpy of sublimation at a given temperature
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>hvapt:</b>	Enthalpy of vaporization at a given temperature
<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>tt:</b>	Triple Point Temperature
<b>vc:</b>	Critical Volume

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