

# 2H-Pyran-2,6(3H)-dione, dihydro-

<b>Other names:</b>	ANHYDRID KYSELINY GLUTAROVE Dihydro-2H-pyran-2,6(3H)-dione GLUTARIC ACID ANHYDRIDE Glutaric anhydride PENTANEDIOIC ANHYDRIDE pentanedioic acid, anhydride
<b>Inchi:</b>	InChI=1S/C5H6O3/c6-4-2-1-3-5(7)8-4/h1-3H2
<b>InchiKey:</b>	VANNPISTIUFMLH-UHFFFAOYSA-N
<b>Formula:</b>	C5H6O3
<b>SMILES:</b>	O=C1CCCC(=O)O1
<b>Mol. weight [g/mol]:</b>	114.10
<b>CAS:</b>	108-55-4

## Physical Properties

Property code	Value	Unit	Source
chs	-2206.50 ± 0.60	kJ/mol	NIST Webbook
gf	-307.92	kJ/mol	Joback Method
hf	-532.40 ± 1.80	kJ/mol	NIST Webbook
hfs	-618.50 ± 0.90	kJ/mol	NIST Webbook
hfus	6.47	kJ/mol	Joback Method
hsub	86.10	kJ/mol	NIST Webbook
hsub	86.10 ± 1.60	kJ/mol	NIST Webbook
hsub	86.10 ± 1.60	kJ/mol	NIST Webbook
hvap	40.47	kJ/mol	Joback Method
ie	11.17	eV	NIST Webbook
log10ws	-0.45		Crippen Method
logp	0.240		Crippen Method
mcvol	79.460	ml/mol	McGowan Method
pc	5109.34	kPa	Joback Method
tb	560.15	K	NIST Webbook
tc	749.54	K	Joback Method
tf	325.15	K	NIST Webbook

tt

329.20

K

Solubility Determination  
and Thermodynamic  
Modeling of Glutaric  
Anhydride in Diverse  
Solvent Systems  
Consisting of Acetic Acid,  
Ethanoic Anhydride, and  
Tetrachloromethane from  
T = (278.45 to 324.45) K

vc

0.284

m<sup>3</sup>/kmol

Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	226.82	J/mol×K	708.05	Joback Method
cpg	171.81	J/mol×K	500.61	Joback Method
cpg	183.79	J/mol×K	542.10	Joback Method
cpg	195.35	J/mol×K	583.59	Joback Method
cpg	206.42	J/mol×K	625.08	Joback Method
cpg	216.93	J/mol×K	666.56	Joback Method
cpg	236.02	J/mol×K	749.54	Joback Method
hsubt	85.90 ± 1.60	kJ/mol	309.00	NIST Webbook
hvapt	60.90	kJ/mol	466.50	NIST Webbook

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	423.20	K	1.30	NIST Webbook
tbrp	440.50 ± 2.50	K	2.70	NIST Webbook

## Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.60108e+01
Coeff. B	-5.80167e+03
Coeff. C	-5.48940e+01

Temperature range (K), min.	423.88
Temperature range (K), max.	597.14

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
Coeff. A	9.65423e+01
Coeff. B	-1.19239e+04
Coeff. C	-1.13780e+01
Coeff. D	4.18011e-06
Temperature range (K), min.	328.00
Temperature range (K), max.	838.00

## 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>KDB:</b>	<a href="https://www.thermochimica.org/files/research/kdb/mol/mol990.mol">https://www.thermochimica.org/files/research/kdb/mol/mol990.mol</a>
<b>KDB Vapor Pressure Data:</b>	<a href="https://www.thermochimica.org/research/kdb/hcprop/showprop.php?cmpid=990">https://www.thermochimica.org/research/kdb/hcprop/showprop.php?cmpid=990</a>
<b>The Yaws Handbook of Vapor Pressure:</b>	<a href="https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure">https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure</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>Solubility Determination and Thermodynamic Modeling of Glutaric Anhydride in Diverse Solvent Systems Consisting of Acetic Acid, Ethanoic Anhydride, and Tetrachloromethane from T = (278.45 to 324.45) K:</b>	<a href="https://www.doi.org/10.1021/acs.jced.8b00496">https://www.doi.org/10.1021/acs.jced.8b00496</a>
<b>NIST Webbook</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C108554&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C108554&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>

## 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>hsub:</b>	Enthalpy of sublimation 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>ie:</b>	Ionization energy
<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>pvap:</b>	Vapor pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tbrp:</b>	Boiling point at reduced pressure
<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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