

# 3,3-Dimethylglutaric acid

<b>Other names:</b>	3,3-Dimethylpentanedioic acid Glutaric acid, 3,3-dimethyl- Pentanedioic acid, 3,3-dimethyl- «beta», «beta»-Dimethylglutaric acid Â«betaÂ»,Â«betaÂ»-Dimethylglutaric acid
<b>Inchi:</b>	InChI=1S/C7H12O4/c1-7(2,3-5(8)9)4-6(10)11/h3-4H2,1-2H3,(H,8,9)(H,10,11)
<b>InchiKey:</b>	DUHQIGLHYXLKAE-UHFFFAOYSA-N
<b>Formula:</b>	C7H12O4
<b>SMILES:</b>	CC(C)(CC(=O)O)CC(=O)O
<b>Mol. weight [g/mol]:</b>	160.17
<b>CAS:</b>	4839-46-7

## Physical Properties

Property code	Value	Unit	Source
gf	-520.58	kJ/mol	Joback Method
hf	-726.18	kJ/mol	Joback Method
hfus	17.85	kJ/mol	Joback Method
hvap	76.73	kJ/mol	Joback Method
log10ws	-0.71		Crippen Method
logp	0.962		Crippen Method
mcvol	124.370	ml/mol	McGowan Method
pc	4103.88	kPa	Joback Method
tb	648.43	K	Joback Method
tc	828.81	K	Joback Method
tf	392.57	K	Joback Method
vc	0.467	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	327.90	J/molxK	648.43	Joback Method
cpg	335.90	J/molxK	678.49	Joback Method
cpg	343.44	J/molxK	708.56	Joback Method
cpg	350.53	J/molxK	738.62	Joback Method

cpg	357.22	J/molxK	768.69	Joback Method
cpg	363.51	J/molxK	798.75	Joback Method
cpg	369.43	J/molxK	828.81	Joback Method
dvisc	0.0046479	Paxs	392.57	Joback Method
dvisc	0.0012880	Paxs	435.21	Joback Method
dvisc	0.0004488	Paxs	477.86	Joback Method
dvisc	0.0001859	Paxs	520.50	Joback Method
dvisc	0.0000880	Paxs	563.14	Joback Method
dvisc	0.0000463	Paxs	605.79	Joback Method
dvisc	0.0000265	Paxs	648.43	Joback Method

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	362.70	K	0.30	NIST Webbook

## Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.77303e+01
Coeff. B	-6.45093e+03
Coeff. C	-1.09965e+02
Temperature range (K), min.	479.80
Temperature range (K), max.	629.41

## Sources

<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>
<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=C4839467&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C4839467&amp;Units=SI</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>

# 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>hvac:</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>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>vc:</b>	Critical Volume

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