

# Butanedioic acid, 2,3-dihydroxy-, [S-(R\*,R\*)]-

<b>Other names:</b>	(+)-L-tartaric acid (-)-tartaric acid (2R,3R)-2,3-dihydroxybutanedioic acid D-Tartaric acid
<b>Inchi:</b>	InChI=1S/C4H6O6/c5-1(3(7)8)2(6)4(9)10/h1-2,5-6H,(H,7,8)(H,9,10)/t1-,2-/m1/s1
<b>InchiKey:</b>	FEWJPZIEWOKRBE-JCYAYHJZSA-N
<b>Formula:</b>	C4H6O6
<b>SMILES:</b>	O=C(O)C(O)C(O)C(=O)O
<b>Mol. weight [g/mol]:</b>	150.09
<b>CAS:</b>	147-71-7

## Physical Properties

Property code	Value	Unit	Source
chs	-1175.00	kJ/mol	NIST Webbook
chs	-1151.00 ± 0.20	kJ/mol	NIST Webbook
gf	-827.20	kJ/mol	Joback Method
hf	-970.53	kJ/mol	Joback Method
hfus	18.62	kJ/mol	Joback Method
hvap	103.93	kJ/mol	Joback Method
log10ws	1.55		Crippen Method
logp	-2.123		Crippen Method
mcvol	93.840	ml/mol	McGowan Method
pc	8386.00	kPa	Joback Method
tb	766.50	K	Joback Method
tc	945.33	K	Joback Method
tf	443.35	K	Solid Liquid Equilibrium of d- and l-Tartaric Acid and Their Importance for Enantioseparation
tf	442.72	K	Research on the application of 7-chloro-quinaldine adducts in 7-chloro-quinaldine separation process

tf	444.00	K	A Novel Co-crystal of (R,R)-1,2-Cyclohexanediol with (R,R)-Tartaric Acid, a Key Structure for Resolution of the Racemic (+-)-trans-Diol in Supercritical Carbon Dioxide, and the Binary Melting Phase Relations.
vc	0.336	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	254.68	J/molxK	766.50	Joback Method
cpg	258.69	J/molxK	796.30	Joback Method
cpg	262.44	J/molxK	826.11	Joback Method
cpg	265.93	J/molxK	855.91	Joback Method
cpg	269.18	J/molxK	885.72	Joback Method
cpg	272.19	J/molxK	915.52	Joback Method
cpg	274.96	J/molxK	945.33	Joback Method
dvisc	0.0013755	Paxs	447.98	Joback Method
dvisc	0.0002009	Paxs	501.07	Joback Method
dvisc	0.0000424	Paxs	554.15	Joback Method
dvisc	0.0000118	Paxs	607.24	Joback Method
dvisc	0.0000040	Paxs	660.33	Joback Method
dvisc	0.0000016	Paxs	713.41	Joback Method
dvisc	0.0000007	Paxs	766.50	Joback Method

## Sources

### Crippen Method:

[https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

Research on the application of 7-chloro-quinoline adducts in a novel co-crystal separation of (R,R)-1,2-Cyclohexanediol with (R,R)-Tartaric Acid. A Key Structure for Resolution of the Racemic (+-)-trans-Diol in Supercritical Carbon Dioxide, and the Binary Melting Phase Relations.:

<https://www.doi.org/10.1016/j.jct.2019.02.002>

<https://www.doi.org/10.1016/j.tca.2009.09.001>

<https://www.doi.org/10.1021/acs.jced.6b01070>

August 31, 2019, 10:00 AM, Kerosene, (+-)-trans-Diol in Supercritical Carbon Dioxide, and the Binary Melting Phase Relations.:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C147717&Units=SI>

<http://link.springer.com/article/10.1007/BF02311772>

### Joback Method:

[https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

Solid Liquid Equilibrium of d- and l-Tartaric Acid and Their Importance for Crystallization:

<https://www.doi.org/10.1021/je300170y>

<http://pubs.acs.org/doi/abs/10.1021/ci990307i>

# Legend

<b>chs:</b>	Standard solid enthalpy of combustion
<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>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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