

# 1,2,4-Butanetricarboxylic acid, 2-hydroxy, trimethyl ester

Inchi:	InChI=1S/C10H16O7/c1-15-7(11)4-5-10(14,9(13)17-3)6-8(12)16-2/h14H,4-6H2,1-3H3
InchiKey:	AACBJIFTOUPSAT-UHFFFAOYSA-N
Formula:	C10H16O7
SMILES:	COC(=O)CCC(O)(CC(=O)OC)C(=O)OC
Mol. weight [g/mol]:	248.23

## Physical Properties

Property code	Value	Unit	Source
gf	-802.42	kJ/mol	Joback Method
hf	-1145.11	kJ/mol	Joback Method
hfus	26.69	kJ/mol	Joback Method
hvap	80.70	kJ/mol	Joback Method
log10ws	0.03		Crippen Method
logp	-0.593		Crippen Method
mcvol	179.950	ml/mol	McGowan Method
pc	2687.42	kPa	Joback Method
rinpol	1443.00		NIST Webbook
tb	746.02	K	Joback Method
tc	935.24	K	Joback Method
tf	482.18	K	Joback Method
vc	0.675	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	513.56	J/molxK	746.02	Joback Method
cpg	523.93	J/molxK	777.56	Joback Method
cpg	533.62	J/molxK	809.09	Joback Method
cpg	542.64	J/molxK	840.63	Joback Method
cpg	550.99	J/molxK	872.17	Joback Method
cpg	558.67	J/molxK	903.70	Joback Method
cpg	565.67	J/molxK	935.24	Joback Method
dvisc	0.0005835	Paxs	482.18	Joback Method
dvisc	0.0002761	Paxs	526.15	Joback Method

dvisc	0.0001466	Paxs	570.13	Joback Method
dvisc	0.0000853	Paxs	614.10	Joback Method
dvisc	0.0000533	Paxs	658.07	Joback Method
dvisc	0.0000353	Paxs	702.05	Joback Method
dvisc	0.0000246	Paxs	746.02	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R106377&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R106377&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>
<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>

## 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>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>rinpol:</b>	Non-polar retention indices
<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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