

# Propionic acid, (2,2,4,4-tetramethylcyclobutane dioxy)bis-

<b>Inchi:</b>	InChI=1S/C14H24O6/c1-13(2)11(19-7-5-9(15)16)14(3,4)12(13)20-8-6-10(17)18/h11-12H
<b>InchiKey:</b>	YJUVIVRSTMYFQ-UHFFFAOYSA-N
<b>Formula:</b>	C14H24O6
<b>SMILES:</b>	CC1(C)C(OCCC(=O)O)C(C)(C)C1OCCC(=O)O
<b>Mol. weight [g/mol]:</b>	288.34
<b>CAS:</b>	97175-20-7

## Physical Properties

Property code	Value	Unit	Source
gf	-659.94	kJ/mol	Joback Method
hf	-1090.25	kJ/mol	Joback Method
hfus	32.42	kJ/mol	Joback Method
hvap	95.28	kJ/mol	Joback Method
log10ws	-1.69		Crippen Method
logp	1.772		Crippen Method
mcvol	223.880	ml/mol	McGowan Method
pc	2183.60	kPa	Joback Method
tb	854.14	K	Joback Method
tc	1050.32	K	Joback Method
tf	563.00	K	Joback Method
vc	0.848	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	737.34	J/molxK	854.14	Joback Method
cpg	753.25	J/molxK	886.84	Joback Method
cpg	769.29	J/molxK	919.53	Joback Method
cpg	785.59	J/molxK	952.23	Joback Method
cpg	802.27	J/molxK	984.93	Joback Method
cpg	819.48	J/molxK	1017.62	Joback Method
cpg	837.34	J/molxK	1050.32	Joback Method

# 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=C97175207&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C97175207&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>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>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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