

# Glutaric acid, but-3-yn-2-yl trans-4-tert-butylcyclohexyl ester

<b>Inchi:</b>	InChI=1S/C19H30O4/c1-6-14(2)22-17(20)8-7-9-18(21)23-16-12-10-15(11-13-16)19(3,4)5
<b>InchiKey:</b>	WIVCEQKUHPDBPG-UHFFFAOYSA-N
<b>Formula:</b>	C19H30O4
<b>SMILES:</b>	<chem>C#CC(C)OC(=O)CCCC(=O)OC1CCC(C(C)(C)C)CC1</chem>
<b>Mol. weight [g/mol]:</b>	322.44

## Physical Properties

Property code	Value	Unit	Source
gf	-118.53	kJ/mol	Joback Method
hf	-613.24	kJ/mol	Joback Method
hfus	35.48	kJ/mol	Joback Method
hvap	74.49	kJ/mol	Joback Method
log10ws	-4.93		Crippen Method
logp	3.870		Crippen Method
mvol	273.990	ml/mol	McGowan Method
pc	1475.88	kPa	Joback Method
rinpol	2176.00		NIST Webbook
rinpol	2176.00		NIST Webbook
tb	788.03	K	Joback Method
tc	999.13	K	Joback Method
tf	485.74	K	Joback Method
vc	1.024	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	855.62	J/mol×K	788.03	Joback Method
cpg	874.71	J/mol×K	823.21	Joback Method
cpg	892.42	J/mol×K	858.40	Joback Method
cpg	908.80	J/mol×K	893.58	Joback Method
cpg	923.89	J/mol×K	928.76	Joback Method
cpg	937.73	J/mol×K	963.95	Joback Method
cpg	950.36	J/mol×K	999.13	Joback Method

# Sources

<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=U393400&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U393400&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</a>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>

# 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>h vap:</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>r in pol:</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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