

# Glutaric acid, 3-methylbut-2-en-1-yl cis-hex-3-enyl ester

<b>Inchi:</b>	InChI=1S/C16H26O4/c1-4-5-6-7-12-19-15(17)9-8-10-16(18)20-13-11-14(2)3/h5-6,11H,4,
<b>InchiKey:</b>	DQZBJDPMNWWDTG-WAYWQWQ TSA-N
<b>Formula:</b>	C16H26O4
<b>SMILES:</b>	CCC=CCCOC(=O)CCCC(=O)OCC=C(C)C
<b>Mol. weight [g/mol]:</b>	282.38

## Physical Properties

Property code	Value	Unit	Source
gf	-232.11	kJ/mol	Joback Method
hf	-638.52	kJ/mol	Joback Method
hfus	41.86	kJ/mol	Joback Method
hvap	69.52	kJ/mol	Joback Method
log10ws	-3.95		Crippen Method
logp	3.566		Crippen Method
mcvol	242.580	ml/mol	McGowan Method
pc	1534.26	kPa	Joback Method
rinpola	1944.00		NIST Webbook
rinpola	1944.00		NIST Webbook
tb	726.26	K	Joback Method
tc	913.61	K	Joback Method
tf	390.28	K	Joback Method
vc	0.941	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	686.64	J/molxK	726.26	Joback Method
cpg	702.33	J/molxK	757.49	Joback Method
cpg	717.21	J/molxK	788.71	Joback Method
cpg	731.29	J/molxK	819.94	Joback Method
cpg	744.60	J/molxK	851.16	Joback Method
cpg	757.18	J/molxK	882.39	Joback Method
cpg	769.05	J/molxK	913.61	Joback Method

# Sources

<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=U394025&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U394025&amp;Units=SI</a>
<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>

# 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>rinpola:</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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