

# Glutaric acid, isohexyl 3-methylbut-2-enyl ester

<b>Inchi:</b>	InChI=1S/C16H28O4/c1-13(2)7-6-11-19-15(17)8-5-9-16(18)20-12-10-14(3)4/h10,13H,5-9
<b>InchiKey:</b>	LTRIEPBFIZMHKL-UHFFFAOYSA-N
<b>Formula:</b>	C16H28O4
<b>SMILES:</b>	CC(C)=CCOC(=O)CCCC(=O)OCCCC(C)C
<b>Mol. weight [g/mol]:</b>	284.39

## Physical Properties

Property code	Value	Unit	Source
gf	-314.77	kJ/mol	Joback Method
hf	-761.02	kJ/mol	Joback Method
hfus	38.14	kJ/mol	Joback Method
hvap	69.17	kJ/mol	Joback Method
log10ws	-3.86		Crippen Method
logp	3.645		Crippen Method
mcvol	246.880	ml/mol	McGowan Method
pc	1482.71	kPa	Joback Method
rinpola	1970.00		NIST Webbook
rinpola	1970.00		NIST Webbook
tb	721.66	K	Joback Method
tc	906.27	K	Joback Method
tf	380.36	K	Joback Method
vc	0.955	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	710.57	J/molxK	721.66	Joback Method
cpg	726.98	J/molxK	752.43	Joback Method
cpg	742.54	J/molxK	783.20	Joback Method
cpg	757.26	J/molxK	813.96	Joback Method
cpg	771.17	J/molxK	844.73	Joback Method
cpg	784.28	J/molxK	875.50	Joback Method
cpg	796.60	J/molxK	906.27	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=U360089&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U360089&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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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