

# Glutaric acid, cyclohexylmethyl isobutyl ester

<b>Inchi:</b>	InChI=1S/C16H28O4/c1-13(2)11-19-15(17)9-6-10-16(18)20-12-14-7-4-3-5-8-14/h13-14H
<b>InchiKey:</b>	HXLONIWEZSABJT-UHFFFAOYSA-N
<b>Formula:</b>	C16H28O4
<b>SMILES:</b>	CC(C)COC(=O)CCCC(=O)OCC1CCCCC1
<b>Mol. weight [g/mol]:</b>	284.39

## Physical Properties

Property code	Value	Unit	Source
gf	-361.99	kJ/mol	Joback Method
hf	-814.13	kJ/mol	Joback Method
hfus	31.08	kJ/mol	Joback Method
hvap	69.56	kJ/mol	Joback Method
log10ws	-3.66		Crippen Method
logp	3.479		Crippen Method
mvol	240.320	ml/mol	McGowan Method
pc	1667.33	kPa	Joback Method
rinpol	1986.00		NIST Webbook
rinpol	1986.00		NIST Webbook
tb	737.17	K	Joback Method
tc	936.26	K	Joback Method
tf	406.78	K	Joback Method
vc	0.906	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	729.43	J/molxK	737.17	Joback Method
cpg	810.88	J/molxK	903.07	Joback Method
cpg	796.88	J/molxK	869.89	Joback Method
cpg	781.74	J/molxK	836.71	Joback Method
cpg	765.47	J/molxK	803.53	Joback Method
cpg	748.04	J/molxK	770.35	Joback Method
cpg	823.77	J/molxK	936.26	Joback Method
dvisc	0.0000892	Paxs	737.17	Joback Method

dvisc	0.0001201	Paxs	682.11	Joback Method
dvisc	0.0001703	Paxs	627.04	Joback Method
dvisc	0.0002585	Paxs	571.97	Joback Method
dvisc	0.0004286	Paxs	516.91	Joback Method
dvisc	0.0008018	Paxs	461.84	Joback Method
dvisc	0.0017773	Paxs	406.78	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U391501&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U391501&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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