

# Glutaric acid, isobutyl 2-methoxyphenyl ester

<b>Inchi:</b>	InChI=1S/C16H22O5/c1-12(2)11-20-15(17)9-6-10-16(18)21-14-8-5-4-7-13(14)19-3/h4-5,
<b>InchiKey:</b>	BDMRUBIAQPLNMS-UHFFFAOYSA-N
<b>Formula:</b>	C16H22O5
<b>SMILES:</b>	COc1ccccc1OC(=O)CCCC(=O)OCC(C)C
<b>Mol. weight [g/mol]:</b>	294.34

## Physical Properties

Property code	Value	Unit	Source
gf	-388.66	kJ/mol	Joback Method
hf	-775.61	kJ/mol	Joback Method
hfus	34.09	kJ/mol	Joback Method
hvap	74.48	kJ/mol	Joback Method
log10ws	-3.46		Crippen Method
logp	2.970		Crippen Method
mcvol	233.290	ml/mol	McGowan Method
pc	1803.09	kPa	Joback Method
rinpola	2156.00		NIST Webbook
tb	771.70	K	Joback Method
tc	975.50	K	Joback Method
tf	460.57	K	Joback Method
vc	0.883	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	676.85	J/molxK	771.70	Joback Method
cpg	691.80	J/molxK	805.67	Joback Method
cpg	705.71	J/molxK	839.63	Joback Method
cpg	718.58	J/molxK	873.60	Joback Method
cpg	730.40	J/molxK	907.57	Joback Method
cpg	741.18	J/molxK	941.54	Joback Method
cpg	750.92	J/molxK	975.50	Joback Method
dvisc	0.0006944	Paxs	460.57	Joback Method
dvisc	0.0003841	Paxs	512.42	Joback Method

dvisc	0.0002368	Paxs	564.28	Joback Method
dvisc	0.0001584	Paxs	616.13	Joback Method
dvisc	0.0001128	Paxs	667.99	Joback Method
dvisc	0.0000844	Paxs	719.85	Joback Method
dvisc	0.0000656	Paxs	771.70	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=U358660&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U358660&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>

## 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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