

# Glutaric acid, 4-chlorobenzyl isobutyl ester

<b>Inchi:</b>	InChI=1S/C16H21ClO4/c1-12(2)10-20-15(18)4-3-5-16(19)21-11-13-6-8-14(17)9-7-13/h6-
<b>InchiKey:</b>	PKCXHPKHAFSP-UHFFFAOYSA-N
<b>Formula:</b>	C16H21ClO4
<b>SMILES:</b>	CC(C)COC(=O)CCCC(=O)OCc1ccc(Cl)cc1
<b>Mol. weight [g/mol]:</b>	312.79

## Physical Properties

Property code	Value	Unit	Source
gf	-295.59	kJ/mol	Joback Method
hf	-659.13	kJ/mol	Joback Method
hfus	37.10	kJ/mol	Joback Method
hvap	76.46	kJ/mol	Joback Method
log10ws	-4.29		Crippen Method
logp	3.753		Crippen Method
mvol	239.660	ml/mol	McGowan Method
pc	1772.85	kPa	Joback Method
rinpol	2261.00		NIST Webbook
rinpol	2261.00		NIST Webbook
tb	786.71	K	Joback Method
tc	995.09	K	Joback Method
tf	468.26	K	Joback Method
vc	0.914	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	675.77	J/molxK	786.71	Joback Method
cpg	689.96	J/molxK	821.44	Joback Method
cpg	703.13	J/molxK	856.17	Joback Method
cpg	715.28	J/molxK	890.90	Joback Method
cpg	726.45	J/molxK	925.63	Joback Method
cpg	736.62	J/molxK	960.36	Joback Method
cpg	745.84	J/molxK	995.09	Joback Method
dvisc	0.0008164	Paxs	468.26	Joback Method

dvisc	0.0004495	Paxs	521.34	Joback Method
dvisc	0.0002763	Paxs	574.41	Joback Method
dvisc	0.0001845	Paxs	627.48	Joback Method
dvisc	0.0001311	Paxs	680.56	Joback Method
dvisc	0.0000980	Paxs	733.63	Joback Method
dvisc	0.0000761	Paxs	786.71	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=U358534&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U358534&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.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>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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