

# Glutaric acid, butyl 3-nitrobenzyl ester

**Inchi:** InChI=1S/C16H21NO6/c1-2-3-10-22-15(18)8-5-9-16(19)23-12-13-6-4-7-14(11-13)17(20)  
**InchiKey:** GOYBXNCRWPDTJH-UHFFFAOYSA-N  
**Formula:** C16H21NO6  
**SMILES:** CCCCOC(=O)CCCC(=O)OCc1cccc([N+](=O)[O-])c1  
**Mol. weight [g/mol]:** 323.34

## Physical Properties

Property code	Value	Unit	Source
gf	-245.67	kJ/mol	Joback Method
hf	-648.87	kJ/mol	Joback Method
hfus	47.78	kJ/mol	Joback Method
hvap	89.05	kJ/mol	Joback Method
log10ws	-4.49		Crippen Method
logp	3.152		Crippen Method
mcvol	244.840	ml/mol	McGowan Method
pc	1835.69	kPa	Joback Method
rinpola	2593.00		NIST Webbook
tb	901.56	K	Joback Method
tc	1124.04	K	Joback Method
tf	596.95	K	Joback Method
vc	0.954	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	754.95	J/mol×K	901.56	Joback Method
cpg	767.04	J/mol×K	938.64	Joback Method
cpg	777.96	J/mol×K	975.72	Joback Method
cpg	787.73	J/mol×K	1012.80	Joback Method
cpg	796.37	J/mol×K	1049.88	Joback Method
cpg	803.89	J/mol×K	1086.96	Joback Method
cpg	810.33	J/mol×K	1124.04	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=U377461&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U377461&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>

# 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>h vap:</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>m cvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>r inpol:</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

Latest version available from:

<https://www.chemeo.com/cid/62-033-6/Glutaric-acid-butyl-3-nitrobenzyl-ester.pdf>

Generated by Cheméo on 2024-04-20 16:03:08.301502323 +0000 UTC m=+15918237.222079639.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.