

# Glutaric acid, 3-methylbut-2-yl 3-nitrobenzyl ester

<b>Inchi:</b>	InChI=1S/C17H23NO6/c1-12(2)13(3)24-17(20)9-5-8-16(19)23-11-14-6-4-7-15(10-14)18(
<b>InchiKey:</b>	BBFQKFFXKPRNDR-UHFFFAOYSA-N
<b>Formula:</b>	C17H23NO6
<b>SMILES:</b>	CC(C)C(C)OC(=O)CCCC(=O)OCc1cccc([N+](=O)[O-])c1
<b>Mol. weight [g/mol]:</b>	337.37

## Physical Properties

Property code	Value	Unit	Source
gf	-242.13	kJ/mol	Joback Method
hf	-680.07	kJ/mol	Joback Method
hfus	43.33	kJ/mol	Joback Method
hvap	90.50	kJ/mol	Joback Method
log10ws	-4.78		Crippen Method
logp	3.396		Crippen Method
mcvol	258.930	ml/mol	McGowan Method
pc	1716.03	kPa	Joback Method
rinpol	2524.00		NIST Webbook
rinpol	2524.00		NIST Webbook
tb	923.56	K	Joback Method
tc	1150.00	K	Joback Method
tf	578.22	K	Joback Method
vc	0.998	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	813.39	J/mol×K	923.56	Joback Method
cpg	825.78	J/mol×K	961.30	Joback Method
cpg	836.89	J/mol×K	999.04	Joback Method
cpg	846.73	J/mol×K	1036.78	Joback Method
cpg	855.34	J/mol×K	1074.52	Joback Method
cpg	862.75	J/mol×K	1112.26	Joback Method
cpg	868.97	J/mol×K	1150.00	Joback Method

# Sources

<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>
<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=U393355&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U393355&amp;Units=SI</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>hvp:</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>rinp:</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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