

# Glutaric acid, isobutyl 4-nitrobenzyl ester

<b>Inchi:</b>	InChI=1S/C16H21NO6/c1-12(2)10-22-15(18)4-3-5-16(19)23-11-13-6-8-14(9-7-13)17(20)
<b>InchiKey:</b>	QLFMNCOMEZDBCX-UHFFFAOYSA-N
<b>Formula:</b>	C16H21NO6
<b>SMILES:</b>	CC(C)COC(=O)CCCC(=O)OCc1ccc([N+](=O)[O-])cc1
<b>Mol. weight [g/mol]:</b>	323.34

## Physical Properties

Property code	Value	Unit	Source
gf	-248.11	kJ/mol	Joback Method
hf	-654.15	kJ/mol	Joback Method
hfus	44.26	kJ/mol	Joback Method
hvap	88.66	kJ/mol	Joback Method
log10ws	-4.25		Crippen Method
logp	3.007		Crippen Method
mcvol	244.840	ml/mol	McGowan Method
pc	1848.33	kPa	Joback Method
rinpola	2494.00		NIST Webbook
rinpola	2494.00		NIST Webbook
tb	901.12	K	Joback Method
tc	1126.06	K	Joback Method
tf	581.95	K	Joback Method
vc	0.948	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	755.49	J/mol×K	901.12	Joback Method
cpg	767.68	J/mol×K	938.61	Joback Method
cpg	778.65	J/mol×K	976.10	Joback Method
cpg	788.44	J/mol×K	1013.59	Joback Method
cpg	797.05	J/mol×K	1051.08	Joback Method
cpg	804.52	J/mol×K	1088.57	Joback Method
cpg	810.87	J/mol×K	1126.06	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U376836&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U376836&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>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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