

# Glutaric acid, 3-nitrobenzyl octyl ester

**Inchi:** InChI=1S/C20H29NO6/c1-2-3-4-5-6-7-14-26-19(22)12-9-13-20(23)27-16-17-10-8-11-18(24)  
**InchiKey:** GNKRTPWJKOVLFY-UHFFFAOYSA-N  
**Formula:** C20H29NO6  
**SMILES:** CCCCCCOC(=O)CCCC(=O)OCc1cccc([N+](=O)[O-])c1  
**Mol. weight [g/mol]:** 379.45

## Physical Properties

Property code	Value	Unit	Source
gf	-211.99	kJ/mol	Joback Method
hf	-731.43	kJ/mol	Joback Method
hfus	58.14	kJ/mol	Joback Method
hvap	97.95	kJ/mol	Joback Method
log10ws	-6.17		Crippen Method
logp	4.712		Crippen Method
mvol	301.200	ml/mol	McGowan Method
pc	1353.63	kPa	Joback Method
rinpol	3015.00		NIST Webbook
tb	993.08	K	Joback Method
tc	1218.94	K	Joback Method
tf	642.03	K	Joback Method
vc	1.177	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	988.43	J/mol×K	993.08	Joback Method
cpg	1001.03	J/mol×K	1030.72	Joback Method
cpg	1012.27	J/mol×K	1068.37	Joback Method
cpg	1022.20	J/mol×K	1106.01	Joback Method
cpg	1030.85	J/mol×K	1143.65	Joback Method
cpg	1038.27	J/mol×K	1181.30	Joback Method
cpg	1044.48	J/mol×K	1218.94	Joback Method

# Sources

<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>
<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=U377466&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U377466&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>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>mccvol:</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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