

# Glutaric acid, decyl 3-methyl-2-nitrobenzyl ester

Inchi:	InChI=1S/C23H35NO6/c1-3-4-5-6-7-8-9-10-17-29-21(25)15-12-16-22(26)30-18-20-14-11
InchiKey:	HZBLBCPNIWVHOS-UHFFFAOYSA-N
Formula:	C23H35NO6
SMILES:	CCCCCCCCCOC(=O)CCCC(=O)OCc1cccc(C)c1[N+](=O)[O-]
Mol. weight [g/mol]:	421.53

## Physical Properties

Property code	Value	Unit	Source
gf	-196.36	kJ/mol	Joback Method
hf	-804.82	kJ/mol	Joback Method
hfus	65.52	kJ/mol	Joback Method
hvap	105.30	kJ/mol	Joback Method
log10ws	-7.48		Crippen Method
logp	5.801		Crippen Method
mcvol	343.470	ml/mol	McGowan Method
pc	1095.72	kPa	Joback Method
rinpola	3095.00		NIST Webbook
tb	1066.70	K	Joback Method
tc	1306.18	K	Joback Method
tf	688.36	K	Joback Method
vc	1.345	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1167.63	J/mol×K	1066.70	Joback Method
cpg	1180.37	J/mol×K	1106.61	Joback Method
cpg	1191.47	J/mol×K	1146.53	Joback Method
cpg	1201.00	J/mol×K	1186.44	Joback Method
cpg	1209.00	J/mol×K	1226.35	Joback Method
cpg	1215.52	J/mol×K	1266.27	Joback Method
cpg	1220.61	J/mol×K	1306.18	Joback Method

# Sources

<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=U376740&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U376740&amp;Units=SI</a>
<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>

# 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>hvac:</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>mccol:</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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