

# Glutaric acid, dodec-9-ynyl propyl ester

**Inchi:** InChI=1S/C20H34O4/c1-3-5-6-7-8-9-10-11-12-13-18-24-20(22)16-14-15-19(21)23-17-4-2  
**InchiKey:** QSAICPKQMDGYFR-UHFFFAOYSA-N  
**Formula:** C20H34O4  
**SMILES:** CCC#CCCCCCCCOC(=O)CCCC(=O)OCCC  
**Mol. weight [g/mol]:** 338.48

## Physical Properties

Property code	Value	Unit	Source
gf	-147.52	kJ/mol	Joback Method
hf	-673.43	kJ/mol	Joback Method
hfus	56.25	kJ/mol	Joback Method
hvap	80.58	kJ/mol	Joback Method
log10ws	-5.71		Crippen Method
logp	4.797		Crippen Method
mcvol	298.940	ml/mol	McGowan Method
pc	1200.62	kPa	Joback Method
rinpol	2462.00		NIST Webbook
rinpol	2462.00		NIST Webbook
tb	818.58	K	Joback Method
tc	1009.33	K	Joback Method
tf	565.58	K	Joback Method
vc	1.165	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	919.80	J/mol×K	818.58	Joback Method
cpg	937.14	J/mol×K	850.37	Joback Method
cpg	953.44	J/mol×K	882.16	Joback Method
cpg	968.72	J/mol×K	913.95	Joback Method
cpg	982.99	J/mol×K	945.75	Joback Method
cpg	996.27	J/mol×K	977.54	Joback Method
cpg	1008.57	J/mol×K	1009.33	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.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=U359784&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U359784&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>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpola:</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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