

# Glutaric acid, hex-4-yn-3-yl nonyl ester

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

## Physical Properties

Property code	Value	Unit	Source
gf	-149.96	kJ/mol	Joback Method
hf	-678.71	kJ/mol	Joback Method
hfus	52.73	kJ/mol	Joback Method
hvap	80.19	kJ/mol	Joback Method
log10ws	-5.83		Crippen Method
logp	4.796		Crippen Method
mvol	298.940	ml/mol	McGowan Method
pc	1207.31	kPa	Joback Method
rmpol	2356.00		NIST Webbook
tb	818.14	K	Joback Method
tc	1010.24	K	Joback Method
tf	550.58	K	Joback Method
vc	1.159	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	920.30	J/mol×K	818.14	Joback Method
cpg	937.76	J/mol×K	850.16	Joback Method
cpg	954.15	J/mol×K	882.17	Joback Method
cpg	969.50	J/mol×K	914.19	Joback Method
cpg	983.82	J/mol×K	946.20	Joback Method
cpg	997.13	J/mol×K	978.22	Joback Method
cpg	1009.43	J/mol×K	1010.24	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=U359860&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U359860&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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