

# Glutaric acid, 3-methylbut-3-enyl propyl ester

<b>Inchi:</b>	InChI=1S/C13H22O4/c1-4-9-16-12(14)6-5-7-13(15)17-10-8-11(2)3/h2,4-10H2,1,3H3
<b>InchiKey:</b>	DAJRVANLOXSFDU-UHFFFAOYSA-N
<b>Formula:</b>	C13H22O4
<b>SMILES:</b>	<chem>C=C(C)CCOC(=O)CCCC(=O)OCCC</chem>
<b>Mol. weight [g/mol]:</b>	242.31

## Physical Properties

Property code	Value	Unit	Source
gf	-329.97	kJ/mol	Joback Method
hf	-685.61	kJ/mol	Joback Method
hfus	32.41	kJ/mol	Joback Method
hvap	62.25	kJ/mol	Joback Method
log10ws	-2.84		Crippen Method
logp	2.619		Crippen Method
mvol	204.610	ml/mol	McGowan Method
pc	1846.75	kPa	Joback Method
rinpol	1678.00		NIST Webbook
rinpol	1678.00		NIST Webbook
tb	645.98	K	Joback Method
tc	827.19	K	Joback Method
tf	364.87	K	Joback Method
vc	0.793	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	545.56	J/molxK	645.98	Joback Method
cpg	560.30	J/molxK	676.18	Joback Method
cpg	574.36	J/molxK	706.38	Joback Method
cpg	587.74	J/molxK	736.58	Joback Method
cpg	600.43	J/molxK	766.79	Joback Method
cpg	612.46	J/molxK	796.99	Joback Method
cpg	623.82	J/molxK	827.19	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U359941&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U359941&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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