

# Glutaric acid, (cyclohex-3-enyl)methyl dec-2-yl ester

Inchi:	InChI=1S/C22H38O4/c1-3-4-5-6-7-9-13-19(2)26-22(24)17-12-16-21(23)25-18-20-14-10-8
InchiKey:	PKTUCXFZABVSON-UHFFFAOYSA-N
Formula:	C22H38O4
SMILES:	CCCCCCCC(C)OC(=O)CCCC(=O)OCC1CC=CCC1
Mol. weight [g/mol]:	366.53

## Physical Properties

Property code	Value	Unit	Source
gf	-281.51	kJ/mol	Joback Method
hf	-880.19	kJ/mol	Joback Method
hfus	47.84	kJ/mol	Joback Method
hvap	83.21	kJ/mol	Joback Method
log10ws	-6.38		Crippen Method
logp	5.739		Crippen Method
mvol	320.560	ml/mol	McGowan Method
pc	1119.30	kPa	Joback Method
rinpol	2551.00		NIST Webbook
rinpol	2551.00		NIST Webbook
tb	873.61	K	Joback Method
tc	1074.57	K	Joback Method
tf	475.16	K	Joback Method
vc	1.228	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1060.87	J/molxK	873.61	Joback Method
cpg	1079.40	J/molxK	907.10	Joback Method
cpg	1096.55	J/molxK	940.60	Joback Method
cpg	1112.36	J/molxK	974.09	Joback Method
cpg	1126.85	J/molxK	1007.58	Joback Method
cpg	1140.05	J/molxK	1041.08	Joback Method
cpg	1152.00	J/molxK	1074.57	Joback Method
dvisc	0.0008638	Paxs	475.16	Joback Method

dvisc	0.0003797	Paxs	541.57	Joback Method
dvisc	0.0001997	Paxs	607.98	Joback Method
dvisc	0.0001193	Paxs	674.38	Joback Method
dvisc	0.0000781	Paxs	740.79	Joback Method
dvisc	0.0000548	Paxs	807.20	Joback Method
dvisc	0.0000406	Paxs	873.61	Joback Method

## Sources

<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=U405532&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U405532&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>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<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>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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