

# Glutaric acid, isohexyl 1-phenyl-2-(3-cyclohexenyl)ethyl ester

Inchi:	InChI=1S/C25H36O4/c1-20(2)11-10-18-28-24(26)16-9-17-25(27)29-23(22-14-7-4-8-15-2
InchiKey:	MULUTUZWDWBARS-UHFFFAOYSA-N
Formula:	C25H36O4
SMILES:	CC(C)CCCOC(=O)CCCC(=O)OC(CC1C=CCCC1)c1ccccc1
Mol. weight [g/mol]:	400.55

## Physical Properties

Property code	Value	Unit	Source
gf	-146.28	kJ/mol	Joback Method
hf	-710.86	kJ/mol	Joback Method
hfus	46.13	kJ/mol	Joback Method
hvap	91.78	kJ/mol	Joback Method
log10ws	-6.84		Crippen Method
logp	6.167		Crippen Method
mcvol	339.070	ml/mol	McGowan Method
pc	1158.50	kPa	Joback Method
rinpola	2902.00		NIST Webbook
tb	968.49	K	Joback Method
tc	1192.00	K	Joback Method
tf	520.39	K	Joback Method
vc	1.282	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1146.61	J/molxK	968.49	Joback Method
cpg	1212.15	J/molxK	1154.75	Joback Method
cpg	1202.06	J/molxK	1117.50	Joback Method
cpg	1190.53	J/molxK	1080.25	Joback Method
cpg	1177.48	J/molxK	1042.99	Joback Method
cpg	1162.86	J/molxK	1005.74	Joback Method
cpg	1220.84	J/molxK	1192.00	Joback Method
dvisc	0.0000242	Paxs	968.49	Joback Method
dvisc	0.0000328	Paxs	893.81	Joback Method

dvisc	0.0000471	Paxs	819.12	Joback Method
dvisc	0.0000727	Paxs	744.44	Joback Method
dvisc	0.0001234	Paxs	669.76	Joback Method
dvisc	0.0002396	Paxs	595.07	Joback Method
dvisc	0.0005624	Paxs	520.39	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=U358588&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U358588&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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