

# Glutaric acid, 2,4-dimethylpent-3-yl isoheptyl ester

Inchi:	InChI=1S/C18H34O4/c1-13(2)9-8-12-21-16(19)10-7-11-17(20)22-18(14(3)4)15(5)6/h13-1
InchiKey:	XXHQGGXDOCDUKX-UHFFFAOYSA-N
Formula:	C18H34O4
SMILES:	CC(C)CCCOC(=O)CCCC(=O)OC(C(C)C)C(C)C
Mol. weight [g/mol]:	314.46

## Physical Properties

Property code	Value	Unit	Source
gf	-376.92	kJ/mol	Joback Method
hf	-925.57	kJ/mol	Joback Method
hfus	33.86	kJ/mol	Joback Method
hvap	72.42	kJ/mol	Joback Method
log10ws	-4.47		Crippen Method
logp	4.360		Crippen Method
mvol	279.360	ml/mol	McGowan Method
pc	1255.70	kPa	Joback Method
rinpol	2011.00		NIST Webbook
rinpol	2011.00		NIST Webbook
tb	762.06	K	Joback Method
tc	946.82	K	Joback Method
tf	376.94	K	Joback Method
vc	1.067	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	851.43	J/molxK	762.06	Joback Method
cpg	931.65	J/molxK	916.03	Joback Method
cpg	917.58	J/molxK	885.24	Joback Method
cpg	902.54	J/molxK	854.44	Joback Method
cpg	886.51	J/molxK	823.65	Joback Method
cpg	869.48	J/molxK	792.85	Joback Method
cpg	944.75	J/molxK	946.82	Joback Method
dvisc	0.0000509	Paxs	762.06	Joback Method

dvisc	0.0000721	Paxs	697.87	Joback Method
dvisc	0.0001097	Paxs	633.69	Joback Method
dvisc	0.0001836	Paxs	569.50	Joback Method
dvisc	0.0003500	Paxs	505.31	Joback Method
dvisc	0.0008051	Paxs	441.13	Joback Method
dvisc	0.0024596	Paxs	376.94	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=U359477&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U359477&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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