

# Glutaric acid, but-3-en-2-yl hept-2-yl ester

<b>Inchi:</b>	InChI=1S/C16H28O4/c1-5-7-8-10-14(4)20-16(18)12-9-11-15(17)19-13(3)6-2/h6,13-14H,2
<b>InchiKey:</b>	LRLGOIWMRYVXRM-UHFFFAOYSA-N
<b>Formula:</b>	C16H28O4
<b>SMILES:</b>	C=CC(C)OC(=O)CCCC(=O)OC(C)CCCC
<b>Mol. weight [g/mol]:</b>	284.39

## Physical Properties

Property code	Value	Unit	Source
gf	-301.04	kJ/mol	Joback Method
hf	-748.30	kJ/mol	Joback Method
hfus	34.44	kJ/mol	Joback Method
hvap	68.08	kJ/mol	Joback Method
log10ws	-4.32		Crippen Method
logp	3.786		Crippen Method
mvol	246.880	ml/mol	McGowan Method
pc	1474.75	kPa	Joback Method
rinpol	1759.00		NIST Webbook
rinpol	1759.00		NIST Webbook
tb	713.86	K	Joback Method
tc	895.86	K	Joback Method
tf	382.64	K	Joback Method
vc	0.949	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	710.01	J/molxK	713.86	Joback Method
cpg	783.88	J/molxK	865.53	Joback Method
cpg	770.77	J/molxK	835.20	Joback Method
cpg	756.84	J/molxK	804.86	Joback Method
cpg	742.08	J/molxK	774.53	Joback Method
cpg	726.47	J/molxK	744.19	Joback Method
cpg	796.17	J/molxK	895.86	Joback Method
dvisc	0.0000837	Paxs	713.86	Joback Method

dvisc	0.0001130	Paxs	658.66	Joback Method
dvisc	0.0001614	Paxs	603.45	Joback Method
dvisc	0.0002476	Paxs	548.25	Joback Method
dvisc	0.0004179	Paxs	493.05	Joback Method
dvisc	0.0008051	Paxs	437.84	Joback Method
dvisc	0.0018739	Paxs	382.64	Joback Method

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U405237&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U405237&amp;Units=SI</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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