

# Glutaric acid, 3-methylbut-2-en-1-yl 3-ethylphenyl ester

Inchi:	InChI=1S/C18H24O4/c1-4-15-7-5-8-16(13-15)22-18(20)10-6-9-17(19)21-12-11-14(2)3/h5
InchiKey:	TWQKWFQSSGZARQ-UHFFFAOYSA-N
Formula:	C18H24O4
SMILES:	CCc1cccc(OC(=O)CCCC(=O)OCC=C(C)C)c1
Mol. weight [g/mol]:	304.38

## Physical Properties

Property code	Value	Unit	Source
gf	-192.71	kJ/mol	Joback Method
hf	-571.96	kJ/mol	Joback Method
hfus	40.49	kJ/mol	Joback Method
hvap	76.95	kJ/mol	Joback Method
log10ws	-4.65		Crippen Method
logp	3.834		Crippen Method
mcvol	251.300	ml/mol	McGowan Method
pc	1624.60	kPa	Joback Method
rinpol	2238.00		NIST Webbook
rinpol	2238.00		NIST Webbook
tb	799.52	K	Joback Method
tc	1006.60	K	Joback Method
tf	456.84	K	Joback Method
vc	0.965	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	735.37	J/molxK	799.52	Joback Method
cpg	750.70	J/molxK	834.03	Joback Method
cpg	765.01	J/molxK	868.55	Joback Method
cpg	778.31	J/molxK	903.06	Joback Method
cpg	790.64	J/molxK	937.57	Joback Method
cpg	802.04	J/molxK	972.09	Joback Method
cpg	812.52	J/molxK	1006.60	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=U390852&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U390852&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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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