

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

<b>Inchi:</b>	InChI=1S/C20H36O4/c1-5-6-7-8-9-10-12-18(4)24-20(22)14-11-13-19(21)23-16-15-17(2)3
<b>InchiKey:</b>	KNTGEIQUIYYLJT-UHFFFAOYSA-N
<b>Formula:</b>	C20H36O4
<b>SMILES:</b>	CCCCCCCCC(C)OC(=O)CCCC(=O)OCC=C(C)C
<b>Mol. weight [g/mol]:</b>	340.50

## Physical Properties

Property code	Value	Unit	Source
gf	-281.09	kJ/mol	Joback Method
hf	-843.58	kJ/mol	Joback Method
hfus	48.50	kJ/mol	Joback Method
hvap	78.08	kJ/mol	Joback Method
log10ws	-5.88		Crippen Method
logp	5.348		Crippen Method
mvol	303.240	ml/mol	McGowan Method
pc	1125.32	kPa	Joback Method
rinpol	2229.00		NIST Webbook
rinpol	2229.00		NIST Webbook
tb	813.18	K	Joback Method
tc	1001.16	K	Joback Method
tf	425.44	K	Joback Method
vc	1.179	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	943.98	J/molxK	813.18	Joback Method
cpg	961.83	J/molxK	844.51	Joback Method
cpg	978.66	J/molxK	875.84	Joback Method
cpg	994.50	J/molxK	907.17	Joback Method
cpg	1009.38	J/molxK	938.50	Joback Method
cpg	1023.31	J/molxK	969.83	Joback Method
cpg	1036.34	J/molxK	1001.16	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=U393507&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U393507&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>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>rinpola:</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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