

# Glutaric acid, tridec-2-yn-1-yl 2-heptyl ester

<b>Inchi:</b>	InChI=1S/C25H44O4/c1-4-6-8-9-10-11-12-13-14-15-17-22-28-24(26)20-18-21-25(27)29-
<b>InchiKey:</b>	FMEUMCOABOBYAB-UHFFFAOYSA-N
<b>Formula:</b>	C25H44O4
<b>SMILES:</b>	CCCCCCCCC#CCOC(=O)CCCC(=O)OC(C)CCCC
<b>Mol. weight [g/mol]:</b>	408.61

## Physical Properties

Property code	Value	Unit	Source
gf	-107.86	kJ/mol	Joback Method
hf	-781.91	kJ/mol	Joback Method
hfus	65.68	kJ/mol	Joback Method
hvap	91.32	kJ/mol	Joback Method
log10ws	-7.92		Crippen Method
logp	6.746		Crippen Method
mvol	369.390	ml/mol	McGowan Method
pc	886.83	kPa	Joback Method
rinpol	2752.00		NIST Webbook
rinpol	2752.00		NIST Webbook
tb	932.54	K	Joback Method
tc	1141.86	K	Joback Method
tf	606.93	K	Joback Method
vc	1.440	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1227.96	J/molxK	932.54	Joback Method
cpg	1247.04	J/molxK	967.43	Joback Method
cpg	1264.68	J/molxK	1002.31	Joback Method
cpg	1280.93	J/molxK	1037.20	Joback Method
cpg	1295.80	J/molxK	1072.09	Joback Method
cpg	1309.35	J/molxK	1106.98	Joback Method
cpg	1321.59	J/molxK	1141.86	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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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=U393589&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U393589&amp;Units=SI</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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