

# Glutaric acid, 2-(adamant-1-yl)ethyl hept-2-yl ester

Inchi:	InChI=1S/C24H40O4/c1-3-4-5-7-18(2)28-23(26)9-6-8-22(25)27-11-10-24-15-19-12-20(16)
InchiKey:	CGVXIGRKJIZGIZ-UHFFFAOYSA-N
Formula:	C24H40O4
SMILES:	CCCCC(C)OC(=O)CCCC(=O)OCCC12CC3CC(CC(C3)C1)C2
Mol. weight [g/mol]:	392.57

## Physical Properties

Property code	Value	Unit	Source
gf	-162.13	kJ/mol	Joback Method
hf	-826.43	kJ/mol	Joback Method
hfus	47.04	kJ/mol	Joback Method
hvap	85.39	kJ/mol	Joback Method
log10ws	-6.42		Crippen Method
logp	5.818		Crippen Method
mvol	331.320	ml/mol	McGowan Method
pc	1114.82	kPa	Joback Method
rmpol	2830.00		NIST Webbook
rmpol	2830.00		NIST Webbook
tb	920.72	K	Joback Method
tc	1131.78	K	Joback Method
tf	559.52	K	Joback Method
vc	1.282	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1177.06	J/molxK	920.72	Joback Method
cpg	1199.93	J/molxK	955.90	Joback Method
cpg	1222.41	J/molxK	991.07	Joback Method
cpg	1244.68	J/molxK	1026.25	Joback Method
cpg	1266.92	J/molxK	1061.43	Joback Method
cpg	1289.32	J/molxK	1096.61	Joback Method
cpg	1312.05	J/molxK	1131.78	Joback Method

# Sources

<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=U405382&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U405382&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>
<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>

# 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>h vap:</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>r in pol:</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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