

# Glutaric acid, hexadecyl 3-methylbut-3-enyl ester

Inchi:	InChI=1S/C26H48O4/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-22-29-25(27)19-18-20-26
InchiKey:	CACVCFGZSQGOLI-UHFFFAOYSA-N
Formula:	C26H48O4
SMILES:	C=C(C)CCOC(=O)CCCC(=O)OCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]:	424.66

## Physical Properties

Property code	Value	Unit	Source
gf	-220.51	kJ/mol	Joback Method
hf	-953.93	kJ/mol	Joback Method
hfus	66.08	kJ/mol	Joback Method
hvap	91.19	kJ/mol	Joback Method
log10ws	-8.28		Crippen Method
logp	7.691		Crippen Method
mcvol	387.780	ml/mol	McGowan Method
pc	782.43	kPa	Joback Method
rinpol	3008.00		NIST Webbook
rinpol	3008.00		NIST Webbook
tb	943.42	K	Joback Method
tc	1159.51	K	Joback Method
tf	511.38	K	Joback Method
vc	1.522	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1315.18	J/molxK	943.42	Joback Method
cpg	1335.85	J/molxK	979.44	Joback Method
cpg	1354.96	J/molxK	1015.45	Joback Method
cpg	1372.58	J/molxK	1051.47	Joback Method
cpg	1388.75	J/molxK	1087.48	Joback Method
cpg	1403.52	J/molxK	1123.50	Joback Method
cpg	1416.95	J/molxK	1159.51	Joback Method

# Sources

<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=U359956&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U359956&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>

# 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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