

# Glutaric acid, hex-4-yn-3-yl 2,4-dichlorophenyl ester

<b>Inchi:</b>	InChI=1S/C17H18Cl2O4/c1-3-6-13(4-2)22-16(20)7-5-8-17(21)23-15-10-9-12(18)11-14(19)
<b>InchiKey:</b>	HOBHANPJNYQAHI-UHFFFAOYSA-N
<b>Formula:</b>	C17H18Cl2O4
<b>SMILES:</b>	CC#CC(CC)OC(=O)CCCC(=O)Oc1ccc(Cl)cc1Cl
<b>Mol. weight [g/mol]:</b>	357.23

## Physical Properties

Property code	Value	Unit	Source
gf	-105.93	kJ/mol	Joback Method
hf	-434.68	kJ/mol	Joback Method
hfus	46.62	kJ/mol	Joback Method
hvap	85.88	kJ/mol	Joback Method
log10ws	-5.69		Crippen Method
logp	4.414		Crippen Method
mcvol	257.390	ml/mol	McGowan Method
pc	1790.91	kPa	Joback Method
rinpola	2445.00		NIST Webbook
rinpola	2445.00		NIST Webbook
tb	861.00	K	Joback Method
tc	1088.30	K	Joback Method
tf	628.07	K	Joback Method
vc	0.982	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	702.74	J/molxK	861.00	Joback Method
cpg	715.15	J/molxK	898.88	Joback Method
cpg	726.43	J/molxK	936.77	Joback Method
cpg	736.59	J/molxK	974.65	Joback Method
cpg	745.64	J/molxK	1012.53	Joback Method
cpg	753.58	J/molxK	1050.42	Joback Method
cpg	760.45	J/molxK	1088.30	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.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=U391851&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U391851&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>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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