

# Glutaric acid, but-3-yn-2-yl 2,6-dichlorophenyl ester

<b>Inchi:</b>	InChI=1S/C15H14Cl2O4/c1-3-10(2)20-13(18)8-5-9-14(19)21-15-11(16)6-4-7-12(15)17/h
<b>InchiKey:</b>	QVRXLWSZMXAFFR-UHFFFAOYSA-N
<b>Formula:</b>	C15H14Cl2O4
<b>SMILES:</b>	C#CC(C)OC(=O)CCCC(=O)Oc1c(Cl)cccc1Cl
<b>Mol. weight [g/mol]:</b>	329.18

## Physical Properties

Property code	Value	Unit	Source
gf	-102.50	kJ/mol	Joback Method
hf	-373.80	kJ/mol	Joback Method
hfus	41.29	kJ/mol	Joback Method
hvap	79.14	kJ/mol	Joback Method
log10ws	-4.85		Crippen Method
logp	3.634		Crippen Method
mcvol	229.210	ml/mol	McGowan Method
pc	2098.42	kPa	Joback Method
rinpola	2173.00		NIST Webbook
rinpola	2173.00		NIST Webbook
tb	796.36	K	Joback Method
tc	1021.30	K	Joback Method
tf	546.40	K	Joback Method
vc	0.870	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	591.18	J/mol×K	796.36	Joback Method
cpg	602.81	J/mol×K	833.85	Joback Method
cpg	613.49	J/mol×K	871.34	Joback Method
cpg	623.21	J/mol×K	908.83	Joback Method
cpg	632.01	J/mol×K	946.32	Joback Method
cpg	639.90	J/mol×K	983.81	Joback Method
cpg	646.89	J/mol×K	1021.30	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=U390251&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U390251&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>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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