

# Glutaric acid, but-3-yn-2-yl 2,4,5-trichlorophenyl ester

<b>Inchi:</b>	InChI=1S/C15H13Cl3O4/c1-3-9(2)21-14(19)5-4-6-15(20)22-13-8-11(17)10(16)7-12(13)18
<b>InchiKey:</b>	KZONOOPTWNEGLX-UHFFFAOYSA-N
<b>Formula:</b>	C15H13Cl3O4
<b>SMILES:</b>	C#CC(C)OC(=O)CCCC(=O)Oc1cc(Cl)c(Cl)cc1Cl
<b>Mol. weight [g/mol]:</b>	363.62

## Physical Properties

Property code	Value	Unit	Source
gf	-124.06	kJ/mol	Joback Method
hf	-401.01	kJ/mol	Joback Method
hfus	45.10	kJ/mol	Joback Method
hvap	84.18	kJ/mol	Joback Method
log10ws	-5.54		Crippen Method
logp	4.287		Crippen Method
mvol	241.450	ml/mol	McGowan Method
pc	2001.91	kPa	Joback Method
rinpol	2368.00		NIST Webbook
rinpol	2368.00		NIST Webbook
tb	838.77	K	Joback Method
tc	1067.32	K	Joback Method
tf	588.84	K	Joback Method
vc	0.918	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	610.69	J/molxK	838.77	Joback Method
cpg	621.10	J/molxK	876.86	Joback Method
cpg	630.55	J/molxK	914.95	Joback Method
cpg	639.05	J/molxK	953.05	Joback Method
cpg	646.62	J/molxK	991.14	Joback Method
cpg	653.27	J/molxK	1029.23	Joback Method
cpg	659.01	J/molxK	1067.32	Joback Method

# Sources

<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=U392156&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U392156&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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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