

# Glutaric acid, 3-methylbut-2-yl 2,5-dichlorophenyl ester

<b>Inchi:</b>	InChI=1S/C16H20Cl2O4/c1-10(2)11(3)21-15(19)5-4-6-16(20)22-14-9-12(17)7-8-13(14)18
<b>InchiKey:</b>	AIZXWQBKDYACHE-UHFFFAOYSA-N
<b>Formula:</b>	C16H20Cl2O4
<b>SMILES:</b>	CC(C)C(C)OC(=O)CCCC(=O)Oc1cc(Cl)ccc1Cl
<b>Mol. weight [g/mol]:</b>	347.23

## Physical Properties

Property code	Value	Unit	Source
gf	-319.59	kJ/mol	Joback Method
hf	-691.62	kJ/mol	Joback Method
hfus	37.38	kJ/mol	Joback Method
hvap	81.12	kJ/mol	Joback Method
log10ws	-5.24		Crippen Method
logp	4.657		Crippen Method
mcvol	251.900	ml/mol	McGowan Method
pc	1708.95	kPa	Joback Method
rinpol	2276.00		NIST Webbook
rinpol	2276.00		NIST Webbook
tb	828.68	K	Joback Method
tc	1044.31	K	Joback Method
tf	495.70	K	Joback Method
vc	0.958	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	700.03	J/molxK	828.68	Joback Method
cpg	713.11	J/molxK	864.62	Joback Method
cpg	725.12	J/molxK	900.56	Joback Method
cpg	736.06	J/molxK	936.49	Joback Method
cpg	745.95	J/molxK	972.43	Joback Method
cpg	754.80	J/molxK	1008.37	Joback Method
cpg	762.63	J/molxK	1044.31	Joback Method
dvisc	0.0006451	Paxs	495.70	Joback Method

dvisc	0.0003577	Paxs	551.20	Joback Method
dvisc	0.0002210	Paxs	606.69	Joback Method
dvisc	0.0001480	Paxs	662.19	Joback Method
dvisc	0.0001054	Paxs	717.69	Joback Method
dvisc	0.0000789	Paxs	773.18	Joback Method
dvisc	0.0000613	Paxs	828.68	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=U392053&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U392053&amp;Units=SI</a>
<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.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>cp<sub>g</sub>:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<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>log<sub>10</sub>ws:</b>	Log <sub>10</sub> of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>m<sub>cvol</sub>:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</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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