

# Glutaric acid, butyl 3,5-dichlorophenyl ester

<b>Inchi:</b>	InChI=1S/C15H18Cl2O4/c1-2-3-7-20-14(18)5-4-6-15(19)21-13-9-11(16)8-12(17)10-13/h
<b>InchiKey:</b>	UCUGNTPTNFKEBJ-UHFFFAOYSA-N
<b>Formula:</b>	C15H18Cl2O4
<b>SMILES:</b>	CCCCOC(=O)CCCC(=O)Oc1cc(Cl)cc(Cl)c1
<b>Mol. weight [g/mol]:</b>	333.21

## Physical Properties

Property code	Value	Unit	Source
gf	-323.13	kJ/mol	Joback Method
hf	-660.42	kJ/mol	Joback Method
hfus	41.84	kJ/mol	Joback Method
hvap	79.67	kJ/mol	Joback Method
log10ws	-4.95		Crippen Method
logp	4.412		Crippen Method
mcvol	237.810	ml/mol	McGowan Method
pc	1827.85	kPa	Joback Method
rinqol	2337.00		NIST Webbook
tb	806.68	K	Joback Method
tc	1018.29	K	Joback Method
tf	514.43	K	Joback Method
vc	0.913	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	643.41	J/molxK	806.68	Joback Method
cpg	696.31	J/molxK	983.02	Joback Method
cpg	687.62	J/molxK	947.76	Joback Method
cpg	678.00	J/molxK	912.49	Joback Method
cpg	667.42	J/molxK	877.22	Joback Method
cpg	655.90	J/molxK	841.95	Joback Method
cpg	704.08	J/molxK	1018.29	Joback Method
dvisc	0.0000837	Paxs	806.68	Joback Method
dvisc	0.0001041	Paxs	757.97	Joback Method

dvisc	0.0001333	Paxs	709.26	Joback Method
dvisc	0.0001771	Paxs	660.56	Joback Method
dvisc	0.0002462	Paxs	611.85	Joback Method
dvisc	0.0003623	Paxs	563.14	Joback Method
dvisc	0.0005736	Paxs	514.43	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=U359440&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U359440&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.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>

## Legend

<b>cpg:</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>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>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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