

# Glutaric acid, 3,5-dichlorophenyl isohexyl ester

Inchi:	InChI=1S/C17H22Cl2O4/c1-12(2)5-4-8-22-16(20)6-3-7-17(21)23-15-10-13(18)9-14(19)1
InchiKey:	ZOOJGHVVGJAEHRW-UHFFFAOYSA-N
Formula:	C17H22Cl2O4
SMILES:	CC(C)CCCOC(=O)CCCC(=O)Oc1cc(Cl)cc(Cl)c1
Mol. weight [g/mol]:	361.26

## Physical Properties

Property code	Value	Unit	Source
gf	-308.73	kJ/mol	Joback Method
hf	-706.98	kJ/mol	Joback Method
hfus	43.49	kJ/mol	Joback Method
hvap	83.73	kJ/mol	Joback Method
log10ws	-5.54		Crippen Method
logp	5.048		Crippen Method
mvol	265.990	ml/mol	McGowan Method
pc	1570.96	kPa	Joback Method
rinpol	2503.00		NIST Webbook
rinpol	2503.00		NIST Webbook
tb	852.00	K	Joback Method
tc	1063.90	K	Joback Method
tf	521.97	K	Joback Method
vc	1.020	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	755.82	J/mol×K	852.00	Joback Method
cpg	768.99	J/mol×K	887.32	Joback Method
cpg	781.08	J/mol×K	922.63	Joback Method
cpg	792.11	J/mol×K	957.95	Joback Method
cpg	802.10	J/mol×K	993.26	Joback Method
cpg	811.05	J/mol×K	1028.58	Joback Method
cpg	818.99	J/mol×K	1063.90	Joback Method
dvisc	0.0005217	Paxs	521.97	Joback Method

dvisc	0.0003039	Paxs	576.98	Joback Method
dvisc	0.0001945	Paxs	631.98	Joback Method
dvisc	0.0001337	Paxs	686.99	Joback Method
dvisc	0.0000971	Paxs	741.99	Joback Method
dvisc	0.0000738	Paxs	797.00	Joback Method
dvisc	0.0000580	Paxs	852.00	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=U359442&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U359442&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>

## 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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