

# Dimethylmalonic acid, isobutyl 2,3,5-trichlorophenyl ester

Inchi:	InChI=1S/C15H17Cl3O4/c1-8(2)7-21-13(19)15(3,4)14(20)22-11-6-9(16)5-10(17)12(11)18
InchiKey:	LFEZGRXARYBFLH-UHFFFAOYSA-N
Formula:	C15H17Cl3O4
SMILES:	CC(C)COC(=O)C(C)(C)C(=O)Oc1cc(Cl)cc(Cl)c1Cl
Mol. weight [g/mol]:	367.65

## Physical Properties

Property code	Value	Unit	Source
gf	-344.29	kJ/mol	Joback Method
hf	-701.66	kJ/mol	Joback Method
hfus	34.71	kJ/mol	Joback Method
hvap	83.03	kJ/mol	Joback Method
log10ws	-5.15		Crippen Method
logp	4.778		Crippen Method
mcvol	250.050	ml/mol	McGowan Method
pc	1789.39	kPa	Joback Method
rinsol	2192.00		NIST Webbook
tb	845.42	K	Joback Method
tc	1072.72	K	Joback Method
tf	544.29	K	Joback Method
vc	0.946	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	666.74	J/molxK	845.42	Joback Method
cpg	714.30	J/molxK	1034.84	Joback Method
cpg	706.76	J/molxK	996.95	Joback Method
cpg	698.26	J/molxK	959.07	Joback Method
cpg	688.78	J/molxK	921.19	Joback Method
cpg	678.28	J/molxK	883.30	Joback Method
cpg	720.91	J/molxK	1072.72	Joback Method
dvisc	0.0000532	Paxs	845.42	Joback Method
dvisc	0.0000672	Paxs	795.23	Joback Method

dvisc	0.0000876	Paxs	745.04	Joback Method
dvisc	0.0001186	Paxs	694.86	Joback Method
dvisc	0.0001685	Paxs	644.67	Joback Method
dvisc	0.0002539	Paxs	594.48	Joback Method
dvisc	0.0004127	Paxs	544.29	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=U363906&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U363906&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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