

# 1,3-Dichloroisopropyl butyrate

<b>Inchi:</b>	InChI=1S/C7H12Cl2O2/c1-3-4-6(10)11-7(2,9)5-8/h3-5H2,1-2H3
<b>InchiKey:</b>	QDOBHQKYXRPNEU-UHFFFAOYSA-N
<b>Formula:</b>	C7H12Cl2O2
<b>SMILES:</b>	CCCC(=O)OC(C)(Cl)CCl
<b>Mol. weight [g/mol]:</b>	199.07

## Physical Properties

Property code	Value	Unit	Source
gf	-246.88	kJ/mol	Joback Method
hf	-472.84	kJ/mol	Joback Method
hfus	17.65	kJ/mol	Joback Method
hvap	47.81	kJ/mol	Joback Method
log10ws	-2.53		Crippen Method
logp	2.524		Crippen Method
mcvol	141.410	ml/mol	McGowan Method
pc	2773.00	kPa	Joback Method
rinpol	1200.00		NIST Webbook
tb	507.48	K	Joback Method
tc	707.27	K	Joback Method
tf	303.07	K	Joback Method
vc	0.538	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	294.12	J/molxK	507.48	Joback Method
cpg	305.33	J/molxK	540.78	Joback Method
cpg	315.93	J/molxK	574.08	Joback Method
cpg	325.92	J/molxK	607.38	Joback Method
cpg	335.33	J/molxK	640.67	Joback Method
cpg	344.19	J/molxK	673.97	Joback Method
cpg	352.51	J/molxK	707.27	Joback Method
dvisc	0.0034763	Paxs	303.07	Joback Method
dvisc	0.0018321	Paxs	337.14	Joback Method

dvisc	0.0010860	Paxs	371.21	Joback Method
dvisc	0.0007029	Paxs	405.28	Joback Method
dvisc	0.0004867	Paxs	439.34	Joback Method
dvisc	0.0003553	Paxs	473.41	Joback Method
dvisc	0.0002706	Paxs	507.48	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R150215&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R150215&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>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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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