

# 2-Ethylbutyric acid, 3,5-dichlorophenyl ester

<b>Inchi:</b>	InChI=1S/C12H14Cl2O2/c1-3-8(4-2)12(15)16-11-6-9(13)5-10(14)7-11/h5-8H,3-4H2,1-2H
<b>InchiKey:</b>	MFBUSXLKRCZXPL-UHFFFAOYSA-N
<b>Formula:</b>	C12H14Cl2O2
<b>SMILES:</b>	CCC(CC)C(=O)Oc1cc(Cl)cc(Cl)c1
<b>Mol. weight [g/mol]:</b>	261.14

## Physical Properties

Property code	Value	Unit	Source
gf	-116.91	kJ/mol	Joback Method
hf	-358.98	kJ/mol	Joback Method
hfus	27.76	kJ/mol	Joback Method
hvap	63.44	kJ/mol	Joback Method
log10ws	-4.59		Crippen Method
logp	4.335		Crippen Method
mcvol	188.100	ml/mol	McGowan Method
pc	2291.52	kPa	Joback Method
rinpol	1667.00		NIST Webbook
rinpol	1667.00		NIST Webbook
tb	661.31	K	Joback Method
tc	880.74	K	Joback Method
tf	393.46	K	Joback Method
vc	0.716	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	446.80	J/molxK	661.31	Joback Method
cpg	459.97	J/molxK	697.88	Joback Method
cpg	472.30	J/molxK	734.45	Joback Method
cpg	483.81	J/molxK	771.02	Joback Method
cpg	494.53	J/molxK	807.59	Joback Method
cpg	504.46	J/molxK	844.17	Joback Method
cpg	513.62	J/molxK	880.74	Joback Method
dvisc	0.0013178	Paxs	393.46	Joback Method

dvisc	0.0007610	Paxs	438.10	Joback Method
dvisc	0.0004865	Paxs	482.74	Joback Method
dvisc	0.0003354	Paxs	527.38	Joback Method
dvisc	0.0002451	Paxs	572.03	Joback Method
dvisc	0.0001874	Paxs	616.67	Joback Method
dvisc	0.0001486	Paxs	661.31	Joback Method

## Sources

<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=U370450&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U370450&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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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