

# 2-Ethylbutyric acid, 2,4,6-trichlorophenyl ester

<b>Inchi:</b>	InChI=1S/C12H13Cl3O2/c1-3-7(4-2)12(16)17-11-9(14)5-8(13)6-10(11)15/h5-7H,3-4H2,1
<b>InchiKey:</b>	BMGWCYDYGBETNN-UHFFFAOYSA-N
<b>Formula:</b>	C12H13Cl3O2
<b>SMILES:</b>	CCC(CC)C(=O)Oc1c(Cl)cc(Cl)cc1Cl
<b>Mol. weight [g/mol]:</b>	295.59

## Physical Properties

Property code	Value	Unit	Source
gf	-138.47	kJ/mol	Joback Method
hf	-386.19	kJ/mol	Joback Method
hfus	31.57	kJ/mol	Joback Method
hvap	68.49	kJ/mol	Joback Method
log10ws	-5.27		Crippen Method
logp	4.988		Crippen Method
mcvol	200.340	ml/mol	McGowan Method
pc	2181.56	kPa	Joback Method
rinsol	1807.00		NIST Webbook
tb	703.72	K	Joback Method
tc	927.03	K	Joback Method
tf	435.90	K	Joback Method
vc	0.764	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	469.65	J/molxK	703.72	Joback Method
cpg	481.68	J/molxK	740.94	Joback Method
cpg	492.90	J/molxK	778.16	Joback Method
cpg	503.31	J/molxK	815.38	Joback Method
cpg	512.94	J/molxK	852.60	Joback Method
cpg	521.80	J/molxK	889.81	Joback Method
cpg	529.90	J/molxK	927.03	Joback Method
dvisc	0.0009519	Paxs	435.90	Joback Method
dvisc	0.0005906	Paxs	480.54	Joback Method

dvisc	0.0003974	Paxs	525.17	Joback Method
dvisc	0.0002845	Paxs	569.81	Joback Method
dvisc	0.0002138	Paxs	614.45	Joback Method
dvisc	0.0001670	Paxs	659.08	Joback Method
dvisc	0.0001346	Paxs	703.72	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=U370159&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U370159&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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