

# Isovaleric acid, 2,4,5-trichlorophenyl ester

<b>Inchi:</b>	InChI=1S/C11H11Cl3O2/c1-6(2)3-11(15)16-10-5-8(13)7(12)4-9(10)14/h4-6H,3H2,1-2H3
<b>InchiKey:</b>	JAPFIXZLXNGZGL-UHFFFAOYSA-N
<b>Formula:</b>	C11H11Cl3O2
<b>SMILES:</b>	CC(C)CC(=O)Oc1cc(Cl)c(Cl)cc1Cl
<b>Mol. weight [g/mol]:</b>	281.56

## Physical Properties

Property code	Value	Unit	Source
gf	-146.89	kJ/mol	Joback Method
hf	-365.55	kJ/mol	Joback Method
hfus	28.97	kJ/mol	Joback Method
hvap	66.27	kJ/mol	Joback Method
log10ws	-4.85		Crippen Method
logp	4.598		Crippen Method
mvol	186.250	ml/mol	McGowan Method
pc	2391.19	kPa	Joback Method
rinpol	1778.00		NIST Webbook
rinpol	1778.00		NIST Webbook
tb	680.84	K	Joback Method
tc	908.18	K	Joback Method
tf	424.63	K	Joback Method
vc	0.709	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	419.54	J/molxK	680.84	Joback Method
cpg	468.84	J/molxK	870.29	Joback Method
cpg	460.48	J/molxK	832.40	Joback Method
cpg	451.37	J/molxK	794.51	Joback Method
cpg	441.52	J/molxK	756.62	Joback Method
cpg	430.91	J/molxK	718.73	Joback Method
cpg	476.48	J/molxK	908.18	Joback Method
dvisc	0.0001517	Paxs	680.84	Joback Method

dvisc	0.0001873	Paxs	638.14	Joback Method
dvisc	0.0002384	Paxs	595.44	Joback Method
dvisc	0.0003149	Paxs	552.74	Joback Method
dvisc	0.0004358	Paxs	510.03	Joback Method
dvisc	0.0006401	Paxs	467.33	Joback Method
dvisc	0.0010158	Paxs	424.63	Joback Method

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U360658&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U360658&amp;Units=SI</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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