

# Ethyl 3-(trichloromethyl)benzoate

<b>Inchi:</b>	InChI=1S/C10H9Cl3O2/c1-2-15-9(14)7-4-3-5-8(6-7)10(11,12)13/h3-6H,2H2,1H3
<b>InchiKey:</b>	OGPQSM AOYBLNQE-UHFFFAOYSA-N
<b>Formula:</b>	C10H9Cl3O2
<b>SMILES:</b>	CCOC(=O)c1cccc(C(Cl)(Cl)Cl)c1
<b>Mol. weight [g/mol]:</b>	267.54
<b>CAS:</b>	116495-76-2

## Physical Properties

Property code	Value	Unit	Source
gf	-130.77	kJ/mol	Joback Method
hf	-325.44	kJ/mol	Joback Method
hfus	23.27	kJ/mol	Joback Method
hvap	61.81	kJ/mol	Joback Method
log10ws	-4.14		Crippen Method
logp	3.690		Crippen Method
mcvol	172.160	ml/mol	McGowan Method
pc	2746.90	kPa	Joback Method
tb	645.21	K	Joback Method
tc	884.19	K	Joback Method
tf	405.74	K	Joback Method
vc	0.647	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	376.75	J/molxK	645.21	Joback Method
cpg	423.59	J/molxK	844.36	Joback Method
cpg	415.86	J/molxK	804.53	Joback Method
cpg	407.37	J/molxK	764.70	Joback Method
cpg	398.05	J/molxK	724.87	Joback Method
cpg	387.87	J/molxK	685.04	Joback Method
cpg	430.61	J/molxK	884.19	Joback Method
dvisc	0.0001612	Paxs	645.21	Joback Method
dvisc	0.0002051	Paxs	605.30	Joback Method

dvisc	0.0002700	Paxs	565.39	Joback Method
dvisc	0.0003706	Paxs	525.48	Joback Method
dvisc	0.0005359	Paxs	485.56	Joback Method
dvisc	0.0008277	Paxs	445.65	Joback Method
dvisc	0.0013925	Paxs	405.74	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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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=C116495762&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C116495762&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>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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