

# Carbonic acid, 2,2,2-trichloroethyl 4-cyanophenyl ester

Inchi:	InChI=1S/C10H6Cl3NO3/c11-10(12,13)6-16-9(15)17-8-3-1-7(5-14)2-4-8/h1-4H,6H2
InchiKey:	RULFGWNYONMCRU-UHFFFAOYSA-N
Formula:	C10H6Cl3NO3
SMILES:	N#Cc1ccc(OC(=O)OCC(Cl)(Cl)Cl)cc1
Mol. weight [g/mol]:	294.52

## Physical Properties

Property code	Value	Unit	Source
gf	-102.59	kJ/mol	Joback Method
hf	-292.78	kJ/mol	Joback Method
hfus	25.97	kJ/mol	Joback Method
hvap	74.70	kJ/mol	Joback Method
log10ws	-4.18		Crippen Method
logp	3.444		Crippen Method
mvol	179.410	ml/mol	McGowan Method
pc	2629.85	kPa	Joback Method
rinpol	1969.00		NIST Webbook
rinpol	1969.00		NIST Webbook
tb	769.71	K	Joback Method
tc	1015.64	K	Joback Method
tf	492.96	K	Joback Method
vc	0.692	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	408.40	J/mol×K	769.71	Joback Method
cpg	416.27	J/mol×K	810.70	Joback Method
cpg	423.32	J/mol×K	851.69	Joback Method
cpg	429.57	J/mol×K	892.68	Joback Method
cpg	435.07	J/mol×K	933.67	Joback Method
cpg	439.84	J/mol×K	974.65	Joback Method
cpg	443.93	J/mol×K	1015.64	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=U357903&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U357903&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>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>rinpola:</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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