

# 2,2,3-Trichloro-n-(4-chlorophenyl)-n-methylpropanamide

<b>Inchi:</b>	InChI=1S/C10H9Cl4NO/c1-15(9(16)10(13,14)6-11)8-4-2-7(12)3-5-8/h2-5H,6H2,1H3
<b>InchiKey:</b>	FUFASTJDAHMATM-UHFFFAOYSA-N
<b>Formula:</b>	C10H9Cl4NO
<b>SMILES:</b>	CN(C(=O)C(Cl)(Cl)CC)c1ccc(Cl)cc1
<b>Mol. weight [g/mol]:</b>	301.00
<b>CAS:</b>	132829-84-6

## Physical Properties

Property code	Value	Unit	Source
gf	73.08	kJ/mol	Joback Method
hf	-141.43	kJ/mol	Joback Method
hfus	29.30	kJ/mol	Joback Method
hvap	65.83	kJ/mol	Joback Method
log10ws	-3.74		Crippen Method
logp	3.716		Crippen Method
mcvol	188.510	ml/mol	McGowan Method
pc	2684.64	kPa	Joback Method
tb	672.66	K	Joback Method
tc	914.11	K	Joback Method
tf	445.90	K	Joback Method
vc	0.697	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	412.04	J/molxK	672.66	Joback Method
cpg	422.68	J/molxK	712.90	Joback Method
cpg	432.32	J/molxK	753.14	Joback Method
cpg	441.05	J/molxK	793.38	Joback Method
cpg	448.98	J/molxK	833.62	Joback Method
cpg	456.20	J/molxK	873.87	Joback Method
cpg	462.80	J/molxK	914.11	Joback Method

# Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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=C132829846&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C132829846&amp;Units=SI</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>mccvol:</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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