

# Dichlorophen, O,O'-(2-trifluoromethylbenzoyl)-

<b>Inchi:</b>	InChI=1S/C29H16Cl2F6O4/c30-18-9-11-24(40-26(38)20-5-1-3-7-22(20)28(32,33)34)16(1
<b>InchiKey:</b>	MMTJMBSWUMNDKL-UHFFFAOYSA-N
<b>Formula:</b>	C29H16Cl2F6O4
<b>SMILES:</b>	O=C(Oc1ccc(Cl)cc1Cc1cc(Cl)ccc1OC(=O)c1ccccc1C(F)(F)F)c1ccccc1C(F)(F)F
<b>Mol. weight [g/mol]:</b>	613.33

## Physical Properties

Property code	Value	Unit	Source
gf	-1069.72	kJ/mol	Joback Method
hf	-1479.83	kJ/mol	Joback Method
hfus	62.32	kJ/mol	Joback Method
hvap	112.81	kJ/mol	Joback Method
log10ws	-11.32		Crippen Method
logp	9.060		Crippen Method
mvol	374.410	ml/mol	McGowan Method
pc	1124.57	kPa	Joback Method
rinpol	3444.00		NIST Webbook
rinpol	3444.00		NIST Webbook
tb	1216.12	K	Joback Method
tc	1488.91	K	Joback Method
tf	809.93	K	Joback Method
vc	1.460	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1148.69	J/molxK	1216.12	Joback Method
cpg	1155.74	J/molxK	1261.59	Joback Method
cpg	1162.12	J/molxK	1307.05	Joback Method
cpg	1168.05	J/molxK	1352.52	Joback Method
cpg	1173.72	J/molxK	1397.98	Joback Method
cpg	1179.33	J/molxK	1443.45	Joback Method
cpg	1185.09	J/molxK	1488.91	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=U355162&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U355162&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>hvp:</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>rinp:</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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