

# Oxetane, 3-methyl-3-(2-chlorophenoxy)methyl

Inchi:	InChI=1S/C10H11ClO2/c1-10(6-12-7-10)13-9-5-3-2-4-8(9)11/h2-5H,6-7H2,1H3
InchiKey:	POCPIHLYUBPFHX-UHFFFAOYSA-N
Formula:	C10H11ClO2
SMILES:	CC1(Oc2ccccc2Cl)COC1
Mol. weight [g/mol]:	198.65

## Physical Properties

Property code	Value	Unit	Source
gf	-23.79	kJ/mol	Joback Method
hf	-222.75	kJ/mol	Joback Method
hfus	18.41	kJ/mol	Joback Method
hvap	51.03	kJ/mol	Joback Method
log10ws	-2.63		Crippen Method
logp	2.508		Crippen Method
mvol	141.120	ml/mol	McGowan Method
pc	3360.64	kPa	Joback Method
rinpol	1598.00		NIST Webbook
tb	557.91	K	Joback Method
tc	800.10	K	Joback Method
tf	358.44	K	Joback Method
vc	0.522	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	323.08	J/mol×K	557.91	Joback Method
cpg	337.44	J/mol×K	598.28	Joback Method
cpg	350.73	J/mol×K	638.64	Joback Method
cpg	363.11	J/mol×K	679.01	Joback Method
cpg	374.74	J/mol×K	719.37	Joback Method
cpg	385.80	J/mol×K	759.74	Joback Method
cpg	396.45	J/mol×K	800.10	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R6803&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R6803&amp;Units=SI</a>
<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>

# 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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