

# Cypermethrin, isomer 1

<b>Inchi:</b>	InChI=1S/C23H21Cl2NO3/c1-23(2)19(12-20(24)25)21(23)22(27)28-14-16(13-26)15-7-6-
<b>InchiKey:</b>	IHURASJUKICJC-UHFFFAOYSA-N
<b>Formula:</b>	C23H21Cl2NO3
<b>SMILES:</b>	CC1(C)C(C=C(Cl)Cl)C1C(=O)OCC(C#N)c1cccc(Oc2cccc2)c1
<b>Mol. weight [g/mol]:</b>	430.32

## Physical Properties

Property code	Value	Unit	Source
gf	237.44	kJ/mol	Joback Method
hf	-150.57	kJ/mol	Joback Method
hfus	46.24	kJ/mol	Joback Method
hvap	100.61	kJ/mol	Joback Method
log10ws	-6.69		Crippen Method
logp	6.220		Crippen Method
mcvol	311.420	ml/mol	McGowan Method
pc	1397.50	kPa	Joback Method
rinpol	2828.00		NIST Webbook
rinpol	2823.00		NIST Webbook
tb	1060.87	K	Joback Method
tc	1317.23	K	Joback Method
tf	632.87	K	Joback Method
vc	1.202	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	982.34	J/molxK	1060.87	Joback Method
cpg	1001.95	J/molxK	1103.60	Joback Method
cpg	1022.17	J/molxK	1146.32	Joback Method
cpg	1043.27	J/molxK	1189.05	Joback Method
cpg	1065.53	J/molxK	1231.78	Joback Method
cpg	1089.19	J/molxK	1274.50	Joback Method
cpg	1114.54	J/molxK	1317.23	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=R566091&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R566091&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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