

# cyhalofop-butyl

<b>Inchi:</b>	InChI=1S/C20H21NO4/c1-3-4-13-23-20(22)15(2)24-17-9-11-19(12-10-17)25-18-7-5-16(1
<b>InchiKey:</b>	UVRKELUMTCYKQA-HNNXBMFYSA-N
<b>Formula:</b>	C20H21NO4
<b>SMILES:</b>	CCCCOC(=O)C(C)Oc1ccc(Oc2ccc(C#N)cc2)cc1
<b>Mol. weight [g/mol]:</b>	339.38

## Physical Properties

Property code	Value	Unit	Source
gf	9.90	kJ/mol	Joback Method
hf	-355.65	kJ/mol	Joback Method
hfus	38.01	kJ/mol	Joback Method
hvap	90.06	kJ/mol	Joback Method
log10ws	-5.06		Crippen Method
logp	4.461		Crippen Method
mcvol	265.700	ml/mol	McGowan Method
pc	1586.01	kPa	Joback Method
rinpol	2581.00		NIST Webbook
tb	943.09	K	Joback Method
tc	1175.47	K	Joback Method
tf	559.65	K	Joback Method
vc	1.020	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	812.81	J/molxK	943.09	Joback Method
cpg	824.54	J/molxK	981.82	Joback Method
cpg	834.85	J/molxK	1020.55	Joback Method
cpg	843.76	J/molxK	1059.28	Joback Method
cpg	851.29	J/molxK	1098.01	Joback Method
cpg	857.45	J/molxK	1136.74	Joback Method
cpg	862.26	J/molxK	1175.47	Joback Method

# Sources

<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=R404072&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R404072&amp;Units=SI</a>
<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>

# 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>h vap:</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>m cvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</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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