

# proclonol, TFA

<b>Inchi:</b>	InChI=1S/C18H13Cl2F3O2/c19-14-7-3-12(4-8-14)17(11-1-2-11,25-16(24)18(21,22)23)13
<b>InchiKey:</b>	RJHYOGGOZYGMJT-UHFFFAOYSA-N
<b>Formula:</b>	C18H13Cl2F3O2
<b>SMILES:</b>	O=C(OC(c1ccc(Cl)cc1)(c1ccc(Cl)cc1)C1CC1)C(F)(F)F
<b>Mol. weight [g/mol]:</b>	389.20

## Physical Properties

Property code	Value	Unit	Source
gf	-469.54	kJ/mol	Joback Method
hf	-774.04	kJ/mol	Joback Method
hfus	33.41	kJ/mol	Joback Method
hvap	74.33	kJ/mol	Joback Method
log10ws	-6.38		Crippen Method
logp	5.753		Crippen Method
mcvol	243.330	ml/mol	McGowan Method
pc	1875.65	kPa	Joback Method
rinpol	2187.00		NIST Webbook
rinpol	2187.00		NIST Webbook
rinpol	2195.00		NIST Webbook
rinpol	2195.00		NIST Webbook
tb	823.80	K	Joback Method
tc	1063.27	K	Joback Method
tf	527.05	K	Joback Method
vc	0.939	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	684.08	J/molxK	823.80	Joback Method
cpg	696.65	J/molxK	863.71	Joback Method
cpg	708.20	J/molxK	903.62	Joback Method
cpg	718.87	J/molxK	943.53	Joback Method
cpg	728.82	J/molxK	983.45	Joback Method
cpg	738.22	J/molxK	1023.36	Joback Method

## Sources

<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=R522160&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R522160&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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>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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