

# Alprenolol, TFA

<b>Inchi:</b>	InChI=1S/C19H21F6NO4/c1-4-7-13-8-5-6-9-15(13)29-11-14(30-17(28)19(23,24)25)10-20
<b>InchiKey:</b>	CFMTYXOXDDMWHX-UHFFFAOYSA-N
<b>Formula:</b>	C19H21F6NO4
<b>SMILES:</b>	<chem>C=CCc1cccc1OCC(CN(C(=O)C(F)(F)F)C(C)C)OC(=O)C(F)(F)F</chem>
<b>Mol. weight [g/mol]:</b>	441.36
<b>CAS:</b>	40435-85-6

## Physical Properties

Property code	Value	Unit	Source
gf	-1225.40	kJ/mol	Joback Method
hf	-1711.79	kJ/mol	Joback Method
hfus	42.54	kJ/mol	Joback Method
hvap	72.24	kJ/mol	Joback Method
log10ws	-5.19		Crippen Method
logp	4.067		Crippen Method
mvol	285.990	ml/mol	McGowan Method
pc	1266.45	kPa	Joback Method
rinpol	1861.00		NIST Webbook
rinpol	1861.00		NIST Webbook
tb	815.76	K	Joback Method
tc	1005.22	K	Joback Method
tf	496.24	K	Joback Method
vc	1.113	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	882.66	J/molxK	815.76	Joback Method
cpg	896.19	J/molxK	847.34	Joback Method
cpg	908.75	J/molxK	878.91	Joback Method
cpg	920.39	J/molxK	910.49	Joback Method
cpg	931.19	J/molxK	942.07	Joback Method
cpg	941.20	J/molxK	973.65	Joback Method
cpg	950.47	J/molxK	1005.22	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=C40435856&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C40435856&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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