

# XMC, TFA

<b>Inchi:</b>	InChI=1S/C12H12F3NO3/c1-7-4-8(2)6-9(5-7)19-11(18)16(3)10(17)12(13,14)15/h4-6H,1-
<b>InchiKey:</b>	CGLLFTAWFYORRL-UHFFFAOYSA-N
<b>Formula:</b>	C12H12F3NO3
<b>SMILES:</b>	Cc1cc(C)cc(OC(=O)N(C)C(=O)C(F)(F)F)c1
<b>Mol. weight [g/mol]:</b>	275.22

## Physical Properties

Property code	Value	Unit	Source
gf	-690.34	kJ/mol	Joback Method
hf	-964.35	kJ/mol	Joback Method
hfus	29.33	kJ/mol	Joback Method
hvap	60.10	kJ/mol	Joback Method
log10ws	-3.56		Crippen Method
logp	2.823		Crippen Method
mcvol	180.480	ml/mol	McGowan Method
pc	2315.84	kPa	Joback Method
rinpol	1478.00		NIST Webbook
rinpol	1493.00		NIST Webbook
rinpol	1478.00		NIST Webbook
rinpol	1493.00		NIST Webbook
tb	647.78	K	Joback Method
tc	844.48	K	Joback Method
tf	435.21	K	Joback Method
vc	0.691	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	475.39	J/molxK	647.78	Joback Method
cpg	487.83	J/molxK	680.56	Joback Method
cpg	499.44	J/molxK	713.35	Joback Method
cpg	510.27	J/molxK	746.13	Joback Method
cpg	520.34	J/molxK	778.91	Joback Method
cpg	529.68	J/molxK	811.70	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=R522180&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R522180&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>

## 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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