

# 1,1,1-Trifluoro-2-propanol

<b>Other names:</b>	1,1,1-Trifluoroisopropanol 1,1,1-Trifluoropropan-2-ol 1,1,1-Trifluoropropanol-2 1-Methyl-2,2,2-trifluoroethanol 2-Propanol, 1,1,1-trifluoro-
<b>Inchi:</b>	InChI=1S/C3H5F3O/c1-2(7)3(4,5)6/h2,7H,1H3
<b>InchiKey:</b>	GILIJDBJZWGBG-UHFFFAOYSA-N
<b>Formula:</b>	C3H5F3O
<b>SMILES:</b>	CC(O)C(F)(F)F
<b>Mol. weight [g/mol]:</b>	114.07
<b>CAS:</b>	374-01-6

## Physical Properties

Property code	Value	Unit	Source
gf	-746.47	kJ/mol	Joback Method
hf	-859.84	kJ/mol	Joback Method
hfus	5.92	kJ/mol	Joback Method
hvap	44.79	kJ/mol	NIST Webbook
hvap	44.80	kJ/mol	NIST Webbook
log10ws	0.30		Aqueous Solubility Prediction Method
logp	0.930		Crippen Method
mvol	64.310	ml/mol	McGowan Method
pc	4316.89	kPa	Joback Method
tb	354.36	K	Joback Method
tc	504.33	K	Joback Method
tf	173.58	K	Joback Method
vc	0.260	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	127.15	J/mol×K	354.36	Joback Method
cpg	133.41	J/mol×K	379.36	Joback Method

cpg	139.35	J/mol×K	404.35	Joback Method
cpg	144.98	J/mol×K	429.35	Joback Method
cpg	150.32	J/mol×K	454.34	Joback Method
cpg	155.37	J/mol×K	479.34	Joback Method
cpg	160.15	J/mol×K	504.33	Joback Method
hvapt	44.20	kJ/mol	312.50	NIST Webbook

## Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.58046e+01
Coeff. B	-3.07220e+03
Coeff. C	-7.35100e+01
Temperature range (K), min.	271.50
Temperature range (K), max.	366.29

## 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>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>Aqueous Solubility Prediction Method:</b>	<a href="http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa">http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa</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=C374016&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C374016&amp;Units=SI</a>
<b>The Yaws Handbook of Vapor Pressure:</b>	<a href="https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure">https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure</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>hvapt:</b>	Enthalpy of vaporization at a given temperature

<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>pvap:</b>	Vapor pressure
<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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