

# 2,2-Dichloro-3,3,3-trifluoropropionic acid, n-propyl ester

Inchi:	InChI=1S/C6H7Cl2F3O2/c1-2-3-13-4(12)5(7,8)6(9,10)11/h2-3H2,1H3
InchiKey:	IIBBYIUDWCQOKV-UHFFFAOYSA-N
Formula:	C6H7Cl2F3O2
SMILES:	CCCOC(=O)C(Cl)(Cl)C(F)(F)F
Mol. weight [g/mol]:	239.02
CAS:	357-49-3

## Physical Properties

Property code	Value	Unit	Source
gf	-836.89	kJ/mol	Joback Method
hf	-1049.28	kJ/mol	Joback Method
hfus	16.89	kJ/mol	Joback Method
hvap	41.83	kJ/mol	Joback Method
log10ws	-2.77		Crippen Method
logp	2.676		Crippen Method
mcvol	132.630	ml/mol	McGowan Method
pc	2715.50	kPa	Joback Method
tb	479.18	K	Joback Method
tc	663.79	K	Joback Method
tf	295.99	K	Joback Method
vc	0.525	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	280.69	J/molxK	479.18	Joback Method
cpg	290.29	J/molxK	509.95	Joback Method
cpg	299.24	J/molxK	540.72	Joback Method
cpg	307.58	J/molxK	571.49	Joback Method
cpg	315.34	J/molxK	602.26	Joback Method
cpg	322.54	J/molxK	633.02	Joback Method
cpg	329.23	J/molxK	663.79	Joback Method

# Sources

<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>
<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=C357493&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C357493&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>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>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical 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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