

# Sulfone, tert-butyl 2-chloroethyl

<b>Inchi:</b>	InChI=1S/C6H13ClO2S/c1-6(2,3)10(8,9)5-4-7/h4-5H2,1-3H3
<b>InchiKey:</b>	ZCOVKORAIYPATP-UHFFFAOYSA-N
<b>Formula:</b>	C6H13ClO2S
<b>SMILES:</b>	CC(C)(C)S(=O)(=O)CCCl
<b>Mol. weight [g/mol]:</b>	184.68
<b>CAS:</b>	98785-33-2

## Physical Properties

Property code	Value	Unit	Source
gf	-477.99	kJ/mol	Joback Method
hf	-645.01	kJ/mol	Joback Method
hfus	19.46	kJ/mol	Joback Method
hvap	50.67	kJ/mol	Joback Method
log10ws	-1.43		Crippen Method
logp	1.439		Crippen Method
mcvol	135.730	ml/mol	McGowan Method
pc	3642.13	kPa	Joback Method
tb	418.66	K	Joback Method
tc	599.81	K	Joback Method
tf	228.28	K	Joback Method
vc	0.535	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	259.41	J/molxK	418.66	Joback Method
cpg	271.84	J/molxK	448.85	Joback Method
cpg	283.68	J/molxK	479.04	Joback Method
cpg	294.94	J/molxK	509.23	Joback Method
cpg	305.63	J/molxK	539.43	Joback Method
cpg	315.78	J/molxK	569.62	Joback Method
cpg	325.38	J/molxK	599.81	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C98785332&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C98785332&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>
<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>

# 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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