

# Benzene, (1,2-dichloro-1,2,2-trifluoroethyl)-3-(fluorosulfon

Inchi:	InChI=1S/C8H4Cl2F4O2S/c9-7(11,8(10,12)13)5-2-1-3-6(4-5)17(14,15)16/h1-4H
InchiKey:	LFRBTEJGNYIGRF-UHFFFAOYSA-N
Formula:	C8H4Cl2F4O2S
SMILES:	O=S(=O)(F)c1cccc(C(F)(Cl)C(F)(F)Cl)c1
Mol. weight [g/mol]:	311.08

## Physical Properties

Property code	Value	Unit	Source
gf	-1146.70	kJ/mol	Joback Method
hf	-1270.16	kJ/mol	Joback Method
hfus	27.39	kJ/mol	Joback Method
hvap	57.89	kJ/mol	Joback Method
log10ws	-4.03		Crippen Method
logp	3.538		Crippen Method
mcvol	159.470	ml/mol	McGowan Method
pc	3337.38	kPa	Joback Method
rinsol	1365.00		NIST Webbook
tb	527.36	K	Joback Method
tc	726.67	K	Joback Method
tf	324.46	K	Joback Method
vc	0.649	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	341.52	J/mol×K	527.36	Joback Method
cpg	352.39	J/mol×K	560.58	Joback Method
cpg	362.35	J/mol×K	593.80	Joback Method
cpg	371.43	J/mol×K	627.01	Joback Method
cpg	379.69	J/mol×K	660.23	Joback Method
cpg	387.18	J/mol×K	693.45	Joback Method
cpg	393.93	J/mol×K	726.67	Joback Method

# Sources

<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=R504182&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R504182&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>

# 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>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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