

# Benzene, (1,2-dichloro-1,2,2-trifluoroethyl)-4-(trifluoromethyl)

Inchi: InChI=1S/C9H4Cl2F6/c10-7(12,9(11,16)17)5-1-3-6(4-2-5)8(13,14)15/h1-4H

InchiKey: ITPINCKUSHHCDC-UHFFFAOYSA-N

Formula: C9H4Cl2F6

SMILES: FC(F)(F)c1ccc(C(F)(Cl)C(F)(F)Cl)cc1

Mol. weight [g/mol]: 297.02

## Physical Properties

Property code	Value	Unit	Source
gf	-1056.52	kJ/mol	Joback Method
hf	-1238.42	kJ/mol	Joback Method
hfus	17.35	kJ/mol	Joback Method
hvap	38.55	kJ/mol	Joback Method
log10ws	-5.01		Crippen Method
logp	4.898		Crippen Method
mvol	149.010	ml/mol	McGowan Method
pc	2372.59	kPa	Joback Method
rinpol	1039.00		NIST Webbook
rinpol	1039.00		NIST Webbook
tb	497.77	K	Joback Method
tc	692.71	K	Joback Method
tf	300.77	K	Joback Method
vc	0.605	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	328.62	J/molxK	497.77	Joback Method
cpg	340.17	J/molxK	530.26	Joback Method
cpg	350.66	J/molxK	562.75	Joback Method
cpg	360.16	J/molxK	595.24	Joback Method
cpg	368.73	J/molxK	627.73	Joback Method
cpg	376.47	J/molxK	660.22	Joback Method
cpg	383.43	J/molxK	692.71	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R504211&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R504211&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>
<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>hvpap:</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>rinppl:</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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