

Benzene, (1,2-dichloro-1,2,2-trifluoroethyl)

Inchi:	InChI=1S/C8H5Cl2F3/c9-7(11,8(10,12)13)6-4-2-1-3-5-6/h1-5H
InchiKey:	HOUGCQGCXPYPDZ-UHFFFAOYSA-N
Formula:	C8H5Cl2F3
SMILES:	FC(F)(Cl)C(F)(Cl)c1ccccc1
Mol. weight [g/mol]:	229.03

Physical Properties

Property code	Value	Unit	Source
gf	-473.72	kJ/mol	Joback Method
hf	-609.23	kJ/mol	Joback Method
hfus	13.32	kJ/mol	Joback Method
hvap	39.41	kJ/mol	Joback Method
log10ws	-3.91		Crippen Method
logp	3.879		Crippen Method
mvol	129.610	ml/mol	McGowan Method
pc	2999.15	kPa	Joback Method
rinpol	1075.00		NIST Webbook
rinpol	1075.00		NIST Webbook
tb	475.33	K	Joback Method
tc	691.32	K	Joback Method
tf	272.79	K	Joback Method
vc	0.505	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	258.23	J/molxK	475.33	Joback Method
cpg	270.16	J/molxK	511.33	Joback Method
cpg	280.97	J/molxK	547.33	Joback Method
cpg	290.73	J/molxK	583.33	Joback Method
cpg	299.52	J/molxK	619.33	Joback Method
cpg	307.44	J/molxK	655.32	Joback Method
cpg	314.55	J/molxK	691.32	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R504157&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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