

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

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

InchiKey: NCKYRTYWJGQGNN-UHFFFAOYSA-N

Formula: C9H4Cl2F6

SMILES: FC(F)(F)c1ccc(C(F)(F)C(F)(Cl)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
mcvol	149.010	ml/mol	McGowan Method
pc	2372.59	kPa	Joback Method
rinpol	1052.00		NIST Webbook
tb	497.77	K	Joback Method
tc	692.71	K	Joback Method
tf	300.77	K	Joback Method
vc	0.605	m3/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

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=R504271&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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