Benzene, (2,2-dichloro-1,1,2-trifluoroethyl)-3-(trifluorometh

Inchi: InChI=1S/C9H4Cl2F6/c10-9(11,17)7(12,13)5-2-1-3-6(4-5)8(14,15)16/h1-4H
InchiKey: KUSGUJQWNRFXCL-UHFFFAOYSA-N
Formula: C9H4Cl2F6
SMILES: FC(F)(F)c1cccc(C(F)(F)C(F)(Cl)Cl)c1
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	1038.00		NIST Webbook
rinpol	1038.00		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/mol×K	497.77	Joback Method
cpg	340.17	J/mol×K	530.26	Joback Method
cpg	350.66	J/mol×K	562.75	Joback Method
cpg	360.16	J/mol×K	595.24	Joback Method
cpg	368.73	J/mol×K	627.73	Joback Method
cpg	376.47	J/mol×K	660.22	Joback Method
cpg	383.43	J/mol×K	692.71	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=R504251&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume