Benzene, (2,2-dichloro-1,1,2-trifluoroethyl)-2,4,5-trifluoro

Inchi: InChI=1S/C8H2Cl2F6/c9-8(10,16)7(14,15)3-1-5(12)6(13)2-4(3)11/h1-2H
InchiKey: JFERBYQAJAGFKW-UHFFFAOYSA-N
Formula: C8H2Cl2F6
SMILES: Fc1cc(F)c(C(F)(F)C(F)(Cl)Cl)cc1F
Mol. weight [g/mol]: 283.00

Physical Properties

Property code	Value	Unit	Source
gf	-1087.04	kJ/mol	Joback Method
hf	-1231.97	kJ/mol	Joback Method
hfus	21.40	kJ/mol	Joback Method
hvap	38.94	kJ/mol	Joback Method
log10ws	-4.90		Crippen Method
logp	4.297		Crippen Method
mcvol	134.920	ml/mol	McGowan Method
pc	2485.07	kPa	Joback Method
rinpol	1026.00		NIST Webbook
rinpol	1026.00		NIST Webbook
tb	488.08	K	Joback Method
tc	676.01	K	Joback Method
tf	312.12	K	Joback Method
vc	0.559	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	283.37	J/mol×K	488.08	Joback Method
cpg	292.40	J/mol×K	519.40	Joback Method
cpg	300.70	J/mol×K	550.72	Joback Method
cpg	308.33	J/mol×K	582.04	Joback Method
cpg	315.32	J/mol×K	613.36	Joback Method
cpg	321.73	J/mol×K	644.69	Joback Method
cpg	327.59	J/mol×K	676.01	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=R504231&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