1,1-dichloro-2,2,2-trifluoro-1-phenylethane

Other names: 1,1,1-Trifluoro-2,2-dichloro-2-phenylethane
Inchi: InChI=1S/C8H5Cl2F3/c9-7(10,8(11,12)13)6-4-2-1-3-5-6/h1-5H
InchiKey: VCGJIIDFWDVVQE-UHFFFAOYSA-N
Formula: C8H5Cl2F3
SMILES: FC(F)(F)C(Cl)(Cl)c1ccccc1
Mol. weight [g/mol]: 229.03
CAS: 309-10-4

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
mcvol	129.610	ml/mol	McGowan Method
pc	2999.15	kPa	Joback Method
tb	363.00 ± 4.00	K	NIST Webbook
tc	691.32	K	Joback Method
tf	272.79	K	Joback Method
vc	0.505	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	258.23	J/mol×K	475.33	Joback Method
cpg	270.16	J/mol×K	511.33	Joback Method
cpg	280.97	J/mol×K	547.33	Joback Method
cpg	290.73	J/mol×K	583.33	Joback Method
cpg	299.52	J/mol×K	619.33	Joback Method
cpg	307.44	J/mol×K	655.32	Joback Method
cpg	314.55	J/mol×K	691.32	Joback Method
hvapt	47.20	kJ/mol	405.50	NIST Webbook

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=C309104&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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume