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

Inchi: InChI=1S/C8H6ClF3/c9-7(8(10,11)12)6-4-2-1-3-5-6/h1-5,7H
InchiKey: GIZBYELHYIBHIR-UHFFFAOYSA-N
Formula: C8H6ClF3
SMILES: FC(F)(F)C(Cl)c1ccccc1
Mol. weight [g/mol]: 194.58

Physical Properties

Property code	Value	Unit	Source
gf	-467.07	kJ/mol	Joback Method
hf	-590.02	kJ/mol	Joback Method
hfus	13.02	kJ/mol	Joback Method
hvap	35.93	kJ/mol	Joback Method
log10ws	-3.55		Crippen Method
logp	3.529		Crippen Method
mcvol	117.370	ml/mol	McGowan Method
pc	3086.42	kPa	Joback Method
rinpol	948.00		NIST Webbook
rinpol	948.00		NIST Webbook
rinpol	948.00		NIST Webbook
tb	440.69	K	Joback Method
tc	641.48	K	Joback Method
tf	225.45	K	Joback Method
vc	0.462	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	229.42	J/mol×K	440.69	Joback Method
cpg	241.46	J/mol×K	474.15	Joback Method
cpg	252.62	J/mol×K	507.62	Joback Method
cpg	262.95	J/mol×K	541.08	Joback Method
cpg	272.50	J/mol×K	574.55	Joback Method
cpg	281.30	J/mol×K	608.01	Joback Method
cpg	289.40	J/mol×K	641.48	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=R345334&Units=SI

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