Benzene, 1-chloro-3-(2,2,2-trifluoroethyl)

Inchi: InChI=1S/C8H6ClF3/c9-7-3-1-2-6(4-7)5-8(10,11)12/h1-4H,5H2
InchiKey: NUCKCUUXOKSESF-UHFFFAOYSA-N
Formula: C8H6ClF3
SMILES: FC(F)(F)Cc1cccc(Cl)c1
Mol. weight [g/mol]: 194.58

Physical Properties

Property code	Value	Unit	Source
gf	-474.26	kJ/mol	Joback Method
hf	-596.21	kJ/mol	Joback Method
hfus	16.15	kJ/mol	Joback Method
hvap	36.98	kJ/mol	Joback Method
log10ws	-3.62		Crippen Method
logp	3.445		Crippen Method
mcvol	117.370	ml/mol	McGowan Method
pc	3009.03	kPa	Joback Method
rinpol	978.00		NIST Webbook
rinpol	978.00		NIST Webbook
rinpol	978.00		NIST Webbook
tb	446.11	K	Joback Method
tc	643.63	K	Joback Method
tf	252.97	K	Joback Method
vc	0.468	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	230.05	J/mol×K	446.11	Joback Method
cpg	241.23	J/mol×K	479.03	Joback Method
cpg	251.64	J/mol×K	511.95	Joback Method
cpg	261.33	J/mol×K	544.87	Joback Method
cpg	270.32	J/mol×K	577.79	Joback Method
cpg	278.66	J/mol×K	610.71	Joback Method
cpg	286.38	J/mol×K	643.63	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=R345354&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
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