Benzene, 1-chloro-4-(1-chloro-2,2,2-trifluoroethyl)

Inchi: InChI=1S/C8H5Cl2F3/c9-6-3-1-5(2-4-6)7(10)8(11,12)13/h1-4,7H

InchiKey: AQHYRPGOKQLFEB-UHFFFAOYSA-N

Formula: C8H5Cl2F3

SMILES: FC(F)(F)C(Cl)c1ccc(Cl)cc1

Mol. weight [g/mol]: 229.03

Physical Properties

Property code	Value	Unit	Source
gf	-488.63	kJ/mol	Joback Method
hf	-617.23	kJ/mol	Joback Method
hfus	16.82	kJ/mol	Joback Method
hvap	40.97	kJ/mol	Joback Method
log10ws	-4.23		Crippen Method
logp	4.182		Crippen Method
mcvol	129.610	ml/mol	McGowan Method
pc	2915.53	kPa	Joback Method
rinpol	1025.00		NIST Webbook
rinpol	1025.00		NIST Webbook
tb	483.10	K	Joback Method
tc	691.45	K	Joback Method
tf	267.89	K	Joback Method
vc	0.510	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	255.35	J/mol×K	483.10	Joback Method
cpg	266.06	J/mol×K	517.83	Joback Method
cpg	275.94	J/mol×K	552.55	Joback Method
cpg	285.03	J/mol×K	587.28	Joback Method
cpg	293.40	J/mol×K	622.00	Joback Method
cpg	301.07	J/mol×K	656.73	Joback Method
cpg	308.11	J/mol×K	691.45	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=R515083&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