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

Inchi: InChI=1S/C8H5BrClF3/c9-7(8(11,12)13)5-1-3-6(10)4-2-5/h1-4,7H
InchiKey: ITNDUQJYMQWYAI-UHFFFAOYSA-N
Formula: C8H5BrClF3
SMILES: FC(F)(F)C(Br)c1ccc(Cl)cc1
Mol. weight [g/mol]: 273.48

Physical Properties

Property code	Value	Unit	Source
gf	-462.38	kJ/mol	Joback Method
hf	-575.16	kJ/mol	Joback Method
hfus	17.91	kJ/mol	Joback Method
hvap	43.03	kJ/mol	Joback Method
log10ws	-4.51		Crippen Method
logp	4.338		Crippen Method
mcvol	134.870	ml/mol	McGowan Method
pc	3280.28	kPa	Joback Method
rinpol	1206.00		NIST Webbook
rinpol	1206.00		NIST Webbook
tb	511.83	K	Joback Method
tc	730.57	K	Joback Method
tf	297.77	K	Joback Method
vc	0.523	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	265.65	J/mol×K	511.83	Joback Method
cpg	276.09	J/mol×K	548.29	Joback Method
cpg	285.64	J/mol×K	584.74	Joback Method
cpg	294.35	J/mol×K	621.20	Joback Method
cpg	302.30	J/mol×K	657.65	Joback Method
cpg	309.54	J/mol×K	694.11	Joback Method
cpg	316.14	J/mol×K	730.57	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=R345369&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