Benzene, (1-chloro-2-fluoroethyl)

Inchi: InChI=1S/C8H8ClF/c9-8(6-10)7-4-2-1-3-5-7/h1-5,8H,6H2
InchiKey: DYJOJBALERNQGT-UHFFFAOYSA-N
Formula: C8H8ClF
SMILES: FCC(Cl)c1ccccc1
Mol. weight [g/mol]: 158.60

Physical Properties

Property code	Value	Unit	Source
gf	-80.29	kJ/mol	Joback Method
hf	-189.05	kJ/mol	Joback Method
hfus	14.27	kJ/mol	Joback Method
hvap	38.86	kJ/mol	Joback Method
log10ws	-2.74		Crippen Method
logp	2.936		Crippen Method
mcvol	113.830	ml/mol	McGowan Method
pc	3345.11	kPa	Joback Method
rinpol	1102.00		NIST Webbook
rinpol	1102.00		NIST Webbook
tb	445.38	K	Joback Method
tc	655.27	K	Joback Method
tf	221.85	K	Joback Method
vc	0.436	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	210.15	J/mol×K	445.38	Joback Method
cpg	222.12	J/mol×K	480.36	Joback Method
cpg	233.34	J/mol×K	515.34	Joback Method
cpg	243.85	J/mol×K	550.33	Joback Method
cpg	253.68	J/mol×K	585.31	Joback Method
cpg	262.86	J/mol×K	620.29	Joback Method
cpg	271.42	J/mol×K	655.27	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=R515063&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