Benzene, 1-fluoro-4-(2-fluoroethyl)

Inchi: InChI=1S/C8H8F2/c9-6-5-7-1-3-8(10)4-2-7/h1-4H,5-6H2
InchiKey: GNVQMGXYKGESKP-UHFFFAOYSA-N
Formula: C8H8F2
SMILES: FCCc1ccc(F)cc1
Mol. weight [g/mol]: 142.15

Physical Properties

Property code	Value	Unit	Source
gf	-270.36	kJ/mol	Joback Method
hf	-375.61	kJ/mol	Joback Method
hfus	16.29	kJ/mol	Joback Method
hvap	34.71	kJ/mol	Joback Method
log10ws	-2.46		Crippen Method
logp	2.338		Crippen Method
mcvol	103.360	ml/mol	McGowan Method
pc	3228.31	kPa	Joback Method
rinpol	940.00		NIST Webbook
rinpol	940.00		NIST Webbook
tb	412.64	K	Joback Method
tc	601.15	K	Joback Method
tf	220.04	K	Joback Method
vc	0.411	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	193.19	J/mol×K	412.64	Joback Method
cpg	204.25	J/mol×K	444.06	Joback Method
cpg	214.75	J/mol×K	475.48	Joback Method
cpg	224.72	J/mol×K	506.90	Joback Method
cpg	234.17	J/mol×K	538.32	Joback Method
cpg	243.11	J/mol×K	569.74	Joback Method
cpg	251.58	J/mol×K	601.15	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R345403&Units=SI
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

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