Benzene, 1-fluoro-3-(2-fluoroethyl)

Inchi: InChI=1S/C8H8ClF/c9-8-3-1-2-7(6-8)4-5-10/h1-3,6H,4-5H2
InchiKey: FKTQNUYOHBHIIR-UHFFFAOYSA-N
Formula: C8H8ClF
SMILES: FCCc1cccc(Cl)c1
Mol. weight [g/mol]: 158.60

Physical Properties

Property code	Value	Unit	Source
gf	-87.48	kJ/mol	Joback Method
hf	-195.24	kJ/mol	Joback Method
hfus	17.41	kJ/mol	Joback Method
hvap	39.91	kJ/mol	Joback Method
log10ws	-2.81		Crippen Method
logp	2.852		Crippen Method
mcvol	113.830	ml/mol	McGowan Method
pc	3257.86	kPa	Joback Method
rinpol	929.00		NIST Webbook
tb	450.80	K	Joback Method
tc	657.16	K	Joback Method
tf	249.37	K	Joback Method
vc	0.443	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	210.60	J/mol×K	450.80	Joback Method
cpg	221.71	J/mol×K	485.19	Joback Method
cpg	232.20	J/mol×K	519.59	Joback Method
cpg	242.07	J/mol×K	553.98	Joback Method
cpg	251.36	J/mol×K	588.38	Joback Method
cpg	260.09	J/mol×K	622.77	Joback Method
cpg	268.28	J/mol×K	657.16	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R515112&Units=SI

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