Benzene, (2-fluoroethyl)-

Inchi: InChI=1S/C8H9F/c9-7-6-8-4-2-1-3-5-8/h1-5H,6-7H2
InchiKey: VEEYKGRLIXCNCZ-UHFFFAOYSA-N
Formula: C8H9F
SMILES: FCCc1ccccc1
Mol. weight [g/mol]: 124.16
CAS: 458-87-7

Physical Properties

Property code	Value	Unit	Source
gf	-65.92	kJ/mol	Joback Method
hf	-168.03	kJ/mol	Joback Method
hfus	13.60	kJ/mol	Joback Method
hvap	34.86	kJ/mol	Joback Method
log10ws	-2.13		Crippen Method
logp	2.199		Crippen Method
mcvol	101.590	ml/mol	McGowan Method
pc	3460.21	kPa	Joback Method
rinpol	924.00		NIST Webbook
rinpol	924.00		NIST Webbook
rinpol	924.00		NIST Webbook
tb	408.39	K	Joback Method
tc	606.19	K	Joback Method
tf	206.93	K	Joback Method
vc	0.394	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	183.61	J/mol×K	408.39	Joback Method
cpg	195.78	J/mol×K	441.36	Joback Method
cpg	207.28	J/mol×K	474.32	Joback Method
cpg	218.14	J/mol×K	507.29	Joback Method
cpg	228.38	J/mol×K	540.26	Joback Method
cpg	238.03	J/mol×K	573.23	Joback Method

cpg	247.11	J/mol×K	606.19	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C458877&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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