Benzene, (1-bromo-2-fluoroethyl)

Inchi: InChI=1S/C8H8BrF/c9-8(6-10)7-4-2-1-3-5-7/h1-5,8H,6H2
InchiKey: AZWJTBRXGIPLHX-UHFFFAOYSA-N
Formula: C8H8BrF
SMILES: FCC(Br)c1ccccc1
Mol. weight [g/mol]: 203.05

Physical Properties

Property code	Value	Unit	Source
gf	-54.04	kJ/mol	Joback Method
hf	-146.98	kJ/mol	Joback Method
hfus	15.36	kJ/mol	Joback Method
hvap	40.91	kJ/mol	Joback Method
log10ws	-3.02		Crippen Method
logp	3.092		Crippen Method
mcvol	119.090	ml/mol	McGowan Method
pc	3796.32	kPa	Joback Method
rinpol	1174.00		NIST Webbook
tb	474.11	K	Joback Method
tc	695.43	K	Joback Method
tf	251.73	K	Joback Method
vc	0.450	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	221.44	J/mol×K	474.11	Joback Method
cpg	233.37	J/mol×K	511.00	Joback Method
cpg	244.46	J/mol×K	547.88	Joback Method
cpg	254.78	J/mol×K	584.77	Joback Method
cpg	264.35	J/mol×K	621.66	Joback Method
cpg	273.22	J/mol×K	658.54	Joback Method
cpg	281.44	J/mol×K	695.43	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=R515038&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

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