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

Inchi: InChI=1S/C9H8F4/c10-5-4-7-2-1-3-8(6-7)9(11,12)13/h1-3,6H,4-5H2
InchiKey: QMWQYBIKMAPQRB-UHFFFAOYSA-N
Formula: C9H8F4
SMILES: FCCc1cccc(C(F)(F)F)c1
Mol. weight [g/mol]: 192.15

Physical Properties

Property code	Value	Unit	Source
gf	-648.72	kJ/mol	Joback Method
hf	-797.22	kJ/mol	Joback Method
hfus	17.62	kJ/mol	Joback Method
hvap	34.00	kJ/mol	Joback Method
log10ws	-3.23		Crippen Method
logp	3.217		Crippen Method
mcvol	120.990	ml/mol	McGowan Method
pc	2693.00	kPa	Joback Method
rinpol	961.00		NIST Webbook
rinpol	961.00		NIST Webbook
rinpol	961.00		NIST Webbook
tb	430.83	K	Joback Method
tc	609.85	K	Joback Method
tf	234.91	K	Joback Method
vc	0.492	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	251.28	J/mol×K	430.83	Joback Method
cpg	263.58	J/mol×K	460.67	Joback Method
cpg	275.16	J/mol×K	490.50	Joback Method
cpg	286.05	J/mol×K	520.34	Joback Method
cpg	296.29	J/mol×K	550.18	Joback Method
cpg	305.90	J/mol×K	580.02	Joback Method
cpg	314.91	J/mol×K	609.85	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=R345329&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