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

Inchi: InChI=1S/C8H6F4/c9-7-3-1-2-6(4-7)5-8(10,11)12/h1-4H,5H2
InchiKey: XEMUQSFXYQZZSO-UHFFFAOYSA-N
Formula: C8H6F4
SMILES: Fc1cccc(CC(F)(F)F)c1
Mol. weight [g/mol]: 178.13

Physical Properties

Property code	Value	Unit	Source
gf	-657.14	kJ/mol	Joback Method
hf	-776.58	kJ/mol	Joback Method
hfus	15.03	kJ/mol	Joback Method
hvap	31.78	kJ/mol	Joback Method
log10ws	-3.27		Crippen Method
logp	2.931		Crippen Method
mcvol	106.900	ml/mol	McGowan Method
pc	2982.79	kPa	Joback Method
rinpol	810.00		NIST Webbook
rinpol	810.00		NIST Webbook
tb	407.95	K	Joback Method
tc	588.22	K	Joback Method
tf	223.64	K	Joback Method
vc	0.436	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	211.74	J/mol×K	407.95	Joback Method
cpg	223.04	J/mol×K	437.99	Joback Method
cpg	233.65	J/mol×K	468.04	Joback Method
cpg	243.61	J/mol×K	498.08	Joback Method
cpg	252.95	J/mol×K	528.13	Joback Method
cpg	261.69	J/mol×K	558.17	Joback Method
cpg	269.86	J/mol×K	588.22	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R345374&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

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