Benzene, 1-fluoro-4-(1-chloro-2,2,2-trifluoroethyl)

Other names: Benzene, m1-fluoro-4-(1-chloro-2,2,2-trifluoroethyl)
Inchi: InChI=1S/C8H5ClF4/c9-7(8(11,12)13)5-1-3-6(10)4-2-5/h1-4,7H
InchiKey: AQLDUNZLECVTNU-UHFFFAOYSA-N
Formula: C8H5ClF4
SMILES: Fc1ccc(C(Cl)C(F)(F)F)cc1
Mol. weight [g/mol]: 212.57

Physical Properties

Property code	Value	Unit	Source
gf	-671.51	kJ/mol	Joback Method
hf	-797.60	kJ/mol	Joback Method
hfus	15.71	kJ/mol	Joback Method
hvap	35.77	kJ/mol	Joback Method
log10ws	-3.88		Crippen Method
logp	3.668		Crippen Method
mcvol	119.140	ml/mol	McGowan Method
pc	2890.51	kPa	Joback Method
rinpol	939.00		NIST Webbook
rinpol	939.00		NIST Webbook
rinpol	939.00		NIST Webbook
tb	444.94	K	Joback Method
tc	636.46	K	Joback Method
tf	238.56	K	Joback Method
vc	0.479	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	238.49	J/mol×K	444.94	Joback Method
cpg	249.46	J/mol×K	476.86	Joback Method
cpg	259.68	J/mol×K	508.78	Joback Method
cpg	269.19	J/mol×K	540.70	Joback Method
cpg	278.02	J/mol×K	572.62	Joback Method
cpg	286.21	J/mol×K	604.54	Joback Method

cpg	293.80	J/mol×K	636.46	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=R345389&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

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