Benzene, 1-chloro-3-fluoro-2-methyl-

Other names: 1-Chloro-3-fluoro-2-methylbenzene
2-Chloro-6-fluorotoluene
Inchi: InChI=1S/C7H6ClF/c1-5-6(8)3-2-4-7(5)9/h2-4H,1H3
InchiKey: FNPVYRJTBXHIPB-UHFFFAOYSA-N
Formula: C7H6ClF
SMILES: Cc1c(F)cccc1Cl
Mol. weight [g/mol]: 144.57
CAS: 443-83-4

Physical Properties

Property code	Value	Unit	Source
gf	-105.53	kJ/mol	Joback Method
hf	-186.07	kJ/mol	Joback Method
hfus	14.43	kJ/mol	Joback Method
hvap	38.34	kJ/mol	Joback Method
log10ws	-2.96		Crippen Method
logp	2.788		Crippen Method
mcvol	99.740	ml/mol	McGowan Method
pc	3581.35	kPa	Joback Method
rinpol	927.50		NIST Webbook
rinpol	927.50		NIST Webbook
rinpol	927.50		NIST Webbook
tb	428.20	K	NIST Webbook
tc	643.30	K	Joback Method
tf	250.62	K	Joback Method
vc	0.387	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	172.66	J/mol×K	432.90	Joback Method
cpg	181.96	J/mol×K	467.97	Joback Method
cpg	190.77	J/mol×K	503.03	Joback Method
cpg	199.10	J/mol×K	538.10	Joback Method

cpg	206.95	J/mol×K	573.17	Joback Method
cpg	214.36	J/mol×K	608.23	Joback Method
cpg	221.33	J/mol×K	643.30	Joback Method
hfust	12.60	kJ/mol	246.00	NIST Webbook

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=C443834&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
hfust:	Enthalpy of fusion at a given temperature
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