3-Chloro-2-fluorotoluene

Other names:	Benzene, 1-chloro-2-fluoro-3-methyl- 2-chloro-3-fluorotoluene
Inchi:	InChI=1S/C7H6ClF/c1-5-3-2-4-6(8)7(5)9/h2-4H,1H3
InchiKey:	LHPJOUKIBAEPMW-UHFFFAOYSA-N
Formula:	C7H6ClF
SMILES:	Cc1cccc(Cl)c1F
Mol. weight [g/mol]:	144.57
CAS:	85089-31-2

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
tb	432.90	K	Joback Method
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

Sources

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=C85089312&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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