2,3,5,6-Tetrafluorotoluene

Other names: Benzene, 1,2,4,5-tetrafluoro-3-methyl-
Inchi: InChI=1S/C7H4F4/c1-3-6(10)4(8)2-5(9)7(3)11/h2H,1H3
InchiKey: POMGTQLCZJZYAM-UHFFFAOYSA-N
Formula: C7H4F4
SMILES: Cc1c(F)c(F)cc(F)c1F
Mol. weight [g/mol]: 164.10
CAS: 5230-78-4

Physical Properties

Property code	Value	Unit	Source
gf	-697.29	kJ/mol	Joback Method
hf	-781.60	kJ/mol	Joback Method
hfus	18.69	kJ/mol	Joback Method
hvap	32.83	kJ/mol	Joback Method
ie	9.16 ± 0.02	eV	NIST Webbook
log10ws	-3.27		Crippen Method
logp	2.551		Crippen Method
mcvol	92.810	ml/mol	McGowan Method
pc	3089.85	kPa	Joback Method
tb	398.70	K	NIST Webbook
tc	577.49	K	Joback Method
tf	247.51	K	Joback Method
vc	0.392	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	176.27	J/mol×K	403.24	Joback Method
cpg	183.67	J/mol×K	432.28	Joback Method
cpg	190.80	J/mol×K	461.32	Joback Method
cpg	197.66	J/mol×K	490.36	Joback Method
cpg	204.26	J/mol×K	519.41	Joback Method
cpg	210.60	J/mol×K	548.45	Joback Method
cpg	216.69	J/mol×K	577.49	Joback Method

hfust	5.84	kJ/mol	233.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5230784&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

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
ie:	Ionization energy
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