2-Fluoro-4-iodotoluene

Other names: Benzene, 2-fluoro-4-iodo-1-methyl-
Inchi: InChI=1S/C7H6FI/c1-5-2-3-6(9)4-7(5)8/h2-4H,1H3
InchiKey: QZLWTFTXGKKCHZ-UHFFFAOYSA-N
Formula: C7H6FI
SMILES: Cc1ccc(I)cc1F
Mol. weight [g/mol]: 236.03
CAS: 39998-81-7

Physical Properties

Property code	Value	Unit	Source
gf	-35.48	kJ/mol	Joback Method
hf	-93.46	kJ/mol	Joback Method
hfus	14.63	kJ/mol	Joback Method
hvap	43.33	kJ/mol	Joback Method
log10ws	-3.43		Crippen Method
logp	2.739		Crippen Method
mcvol	113.320	ml/mol	McGowan Method
pc	3646.53	kPa	Joback Method
tb	488.61	K	Joback Method
tc	729.14	K	Joback Method
tf	278.76	K	Joback Method
vc	0.425	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	190.78	J/mol×K	488.61	Joback Method
cpg	200.25	J/mol×K	528.70	Joback Method
cpg	209.06	J/mol×K	568.79	Joback Method
cpg	217.26	J/mol×K	608.88	Joback Method
cpg	224.87	J/mol×K	648.96	Joback Method
cpg	231.93	J/mol×K	689.05	Joback Method
cpg	238.48	J/mol×K	729.14	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C39998817&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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