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

Physical Properties

Property code	Value	Unit	Source
hfus	14.63	kJ/mol	Joback Method
ie	8.56	eV	Cheméo Relay (1.0)
logp	2.739		Crippen Method
mcvol	113.320	ml/mol	McGowan Method
tb	479.25	K	Cheméo Relay (1.0)

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

Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C39998817&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature