2-Fluoro-6-iodobenzonitrile

Inchi: InChI=1S/C7H3FIN/c8-6-2-1-3-7(9)5(6)4-10/h1-3H
InchiKey: FAACTMVXBNSPJA-UHFFFAOYSA-N
Formula: C7H3FIN
SMILES: N#Cc1c(F)cccc1I
Mol. weight [g/mol]: 247.01
CAS: 79544-29-9

Physical Properties

Property code	Value	Unit	Source
gf	97.70	kJ/mol	Joback Method
hf	71.42	kJ/mol	Joback Method
hfus	16.14	kJ/mol	Joback Method
hvap	53.81	kJ/mol	Joback Method
log10ws	-3.30		Crippen Method
logp	2.302		Crippen Method
mcvol	114.700	ml/mol	McGowan Method
pc	3538.87	kPa	Joback Method
tb	590.69	K	Joback Method
tc	848.63	K	Joback Method
tf	343.75	K	Joback Method
vc	0.452	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	201.61	J/mol×K	590.69	Joback Method
cpg	208.55	J/mol×K	633.68	Joback Method
cpg	214.91	J/mol×K	676.67	Joback Method
cpg	220.74	J/mol×K	719.66	Joback Method
cpg	226.08	J/mol×K	762.65	Joback Method
cpg	230.97	J/mol×K	805.64	Joback Method
cpg	235.45	J/mol×K	848.63	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=C79544299&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