5-Fluoro-2-methylbenzonitrile

Inchi: InChI=1S/C8H6FN/c1-6-2-3-8(9)4-7(6)5-10/h2-4H,1H3
InchiKey: IBRODYNXELBTJC-UHFFFAOYSA-N
Formula: C8H6FN
SMILES: Cc1ccc(F)cc1C#N
Mol. weight [g/mol]: 135.14
CAS: 77532-79-7

Physical Properties

Property code	Value	Unit	Source
gf	48.00	kJ/mol	Joback Method
hf	-26.09	kJ/mol	Joback Method
hfus	14.32	kJ/mol	Joback Method
hvap	46.66	kJ/mol	Joback Method
log10ws	-2.63		Crippen Method
logp	2.006		Crippen Method
mcvol	102.970	ml/mol	McGowan Method
pc	3246.73	kPa	Joback Method
tb	520.43	K	Joback Method
tc	742.34	K	Joback Method
tf	296.96	K	Joback Method
vc	0.419	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	208.84	J/mol×K	520.43	Joback Method
cpg	217.98	J/mol×K	557.41	Joback Method
cpg	226.59	J/mol×K	594.40	Joback Method
cpg	234.68	J/mol×K	631.38	Joback Method
cpg	242.27	J/mol×K	668.37	Joback Method
cpg	249.38	J/mol×K	705.35	Joback Method
cpg	256.03	J/mol×K	742.34	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C77532797&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