Benzonitrile, 2-fluoro-6-methoxy-

Other names: 2-fluoro-6-methoxybenzonitrile
Inchi: InChI=1S/C8H6FNO/c1-11-8-4-2-3-7(9)6(8)5-10/h2-4H,1H3
InchiKey: YPMSIWYNTPSPMV-UHFFFAOYSA-N
Formula: C8H6FNO
SMILES: COc1cccc(F)c1C#N
Mol. weight [g/mol]: 151.14
CAS: 94088-46-7

Physical Properties

Property code	Value	Unit	Source
gf	-57.00	kJ/mol	Joback Method
hf	-158.31	kJ/mol	Joback Method
hfus	15.51	kJ/mol	Joback Method
hvap	49.07	kJ/mol	Joback Method
log10ws	-2.28		Crippen Method
logp	1.706		Crippen Method
mcvol	108.840	ml/mol	McGowan Method
pc	3184.73	kPa	Joback Method
tb	542.85	K	Joback Method
tc	762.20	K	Joback Method
tf	319.19	K	Joback Method
vc	0.438	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	229.58	J/mol×K	542.85	Joback Method
cpg	238.65	J/mol×K	579.41	Joback Method
cpg	247.24	J/mol×K	615.97	Joback Method
cpg	255.37	J/mol×K	652.52	Joback Method
cpg	263.04	J/mol×K	689.08	Joback Method
cpg	270.23	J/mol×K	725.64	Joback Method
cpg	276.96	J/mol×K	762.20	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C94088467&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