Benzonitrile, 3-fluoro-

Other names: Benzonitrile, m-fluoro-
m-Cyanofluorobenzene
m-Fluorobenzonitrile
3-Fluorobenzonitrile
Inchi: InChI=1S/C7H4FN/c8-7-3-1-2-6(4-7)5-9/h1-4H
InchiKey: JZTPKAROPNTQQV-UHFFFAOYSA-N
Formula: C7H4FN
SMILES: N#Cc1cccc(F)c1
Mol. weight [g/mol]: 121.11
CAS: 403-54-3

Physical Properties

Property code	Value	Unit	Source
gf	49.21	kJ/mol	Joback Method
hf	6.02	kJ/mol	Joback Method
hfus	12.12	kJ/mol	Joback Method
hvap	43.78	kJ/mol	Joback Method
ie	9.79	eV	NIST Webbook
ie	10.03 ± 0.05	eV	NIST Webbook
ie	9.79	eV	NIST Webbook
log10ws	-2.16		Crippen Method
logp	1.697		Crippen Method
mcvol	88.880	ml/mol	McGowan Method
pc	3699.95	kPa	Joback Method
tb	455.50 ± 0.50	K	NIST Webbook
tc	717.07	K	Joback Method
tf	273.17	K	Joback Method
vc	0.363	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	169.19	J/mol×K	492.57	Joback Method
cpg	177.42	J/mol×K	529.99	Joback Method

cpg	185.12	J/mol×K	567.40	Joback Method
cpg	192.30	J/mol×K	604.82	Joback Method
cpg	198.98	J/mol×K	642.24	Joback Method
cpg	205.20	J/mol×K	679.66	Joback Method
cpg	210.97	J/mol×K	717.07	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	455.70	K	100.00	NIST Webbook

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=C403543&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
ie: Ionization energy
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
tbrp: Boiling point at reduced pressure
tc: Critical Temperature
tf: Normal melting (fusion) point

vc: Critical Volume