

Benzonitrile, 2-fluoro-

Other names:	Benzonitrile, o-fluoro- o-Cyanofluorobenzene o-Fluorobenzonitrile 2-Fluorobenzonitrile
Inchi:	InChI=1S/C7H4FN/c8-7-4-2-1-3-6(7)5-9/h1-4H
InchiKey:	GDHXJNRAJRCGMX-UHFFFAOYSA-N
Formula:	C7H4FN
SMILES:	N#Cc1ccccc1F
Mol. weight [g/mol]:	121.11
CAS:	394-47-8

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	9.78	eV	NIST Webbook
ie	9.78	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	492.57	K	Joback Method
tc	717.07	K	Joback Method
tf	273.17	K	Joback Method
vc	0.363	m ³ /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	363.20	K	2.80	NIST Webbook
tbrp	363.00	K	2.80	NIST Webbook
tbrp	366.50 ± 1.50	K	2.90	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C394478&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
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

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