Benzaldehyde, 2-fluoro-

Other names:	Benzaldehyde, o-fluoro-
	o-Fluorobenzaldehyde
	2-Fluorobenzaldehyde
	ortho-Fluorobenzaldehyde
Inchi:	InChI=1S/C7H5FO/c8-7-4-2-1-3-6(7)5-9/h1-5H
InchiKey:	ZWDVQMVZZYIAHO-UHFFFAOYSA-N
Formula:	C7H5FO
SMILES:	O=Cc1ccccc1F
Mol. weight [g/mol]:	124.11
CAS:	446-52-6

Physical Properties

Property code	Value	Unit	Source
ea	0.64 ± 0.04	eV	NIST Webbook
gf	-183.49	kJ/mol	Joback Method
hf	-244.44	kJ/mol	Joback Method
hfus	12.91	kJ/mol	Joback Method
hvap	40.02	kJ/mol	Joback Method
log10ws	-2.04		Crippen Method
logp	1.638		Crippen Method
mcvol	89.070	ml/mol	McGowan Method
pc	4189.32	kPa	Joback Method
rinpol	941.50		NIST Webbook
rinpol	947.30		NIST Webbook
rinpol	931.00		NIST Webbook
rinpol	941.50		NIST Webbook
tb	448.20	K	NIST Webbook
tc	647.38	K	Joback Method
tf	250.18	K	Joback Method
vc	0.354	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	164.02	J/mol×K	439.15	Joback Method
cpg	173.14	J/mol×K	473.86	Joback Method
cpg	181.71	J/mol×K	508.56	Joback Method
cpg	189.77	J/mol×K	543.27	Joback Method
cpg	197.34	J/mol×K	577.97	Joback Method
cpg	204.42	J/mol×K	612.68	Joback Method
cpg	211.05	J/mol×K	647.38	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	343.00	K	2.70	NIST Webbook
tbrp	363.70	K	6.10	NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C446526&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg: Ideal gas heat capacity
ea: Electron affinity
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
rinpol: Non-polar retention indices

tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume