Benzenamine, 2-fluoro-

Other names:	Aniline, o-fluoro-
	o-Fluoroaniline
	2-Fluoroaniline
	2-Fluorobenzenamine
	1-Amino-2-fluorobenzene
	Aniline, 2-fluoro-
	UN 2941
	Benzeneamine, 2-fluoro
Inchi:	InChI=1S/C6H6FN/c7-5-3-1-2-4-6(5)8/h1-4H,8H2
InchiKey:	FTZQXOJYPFINKJ-UHFFFAOYSA-N
Formula:	C6H6FN
SMILES:	Nc1ccccc1F
Mol. weight [g/mol]:	111.12
CAS:	348-54-9

Physical Properties

Property code	Value	Unit	Source
chl	-3255.80	kJ/mol	NIST Webbook
gf	-25.94	kJ/mol	Joback Method
hf	-104.43	kJ/mol	Joback Method
hfus	13.22	kJ/mol	Joback Method
hvap	52.00 ± 0.60	kJ/mol	NIST Webbook
ie	8.18	eV	NIST Webbook
ie	8.50	eV	NIST Webbook
ie	8.18	eV	NIST Webbook
log10ws	-1.44		Crippen Method
logp	1.408		Crippen Method
mcvol	83.390	ml/mol	McGowan Method
pc	4652.99	kPa	Joback Method
rinpol	929.50		NIST Webbook
rinpol	929.50		NIST Webbook
rinpol	930.00		NIST Webbook
tb	455.70	K	NIST Webbook
tc	658.85	K	Joback Method
tf	280.17	K	Joback Method
vc	0.310	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	157.82	J/mol×K	440.14	Joback Method
cpg	167.25	J/mol×K	476.59	Joback Method
cpg	176.10	J/mol×K	513.04	Joback Method
cpg	184.40	J/mol×K	549.50	Joback Method
cpg	192.17	J/mol×K	585.95	Joback Method
cpg	199.43	J/mol×K	622.40	Joback Method
cpg	206.21	J/mol×K	658.85	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	328.50 ± 0.50	K	1.60	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=C348549&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chl: Standard liquid enthalpy of combustion
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
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