Formamide, N-phenyl-

Other names:	Aniline, N-formyl-
	CARBANILALDEHYDE
	FORMAMIDOBENZENE
	Formanilide
	Formylaniline
	N-Formylaniline
	N-PHENYLFORMAMIDE
	Phenyl formamide
Inchi:	InChI=1S/C7H7NO/c9-6-8-7-4-2-1-3-5-7/h1-6H,(H,8,9)
InchiKey:	DYDNPESBYVVLBO-UHFFFAOYSA-N
Formula:	C7H7NO
SMILES:	O=CNc1ccccc1
Mol. weight [g/mol]:	121.14
CAS:	103-70-8

Physical Properties

Property code	Value	Unit	Source
gf	110.34	kJ/mol	Joback Method
hf	16.61	kJ/mol	Joback Method
hfus	15.31	kJ/mol	Joback Method
hvap	46.61	kJ/mol	Joback Method
ie	8.60	eV	NIST Webbook
log10ws	-0.68		Aqueous Solubility Prediction Method
logp	1.255		Crippen Method
mcvol	97.280	ml/mol	McGowan Method
pc	4615.13	kPa	Joback Method
rinpol	1221.00		NIST Webbook
rinpol	1220.00		NIST Webbook
rinpol	1221.00		NIST Webbook
rinpol	1210.00		NIST Webbook
rinpol	1220.00		NIST Webbook
rinpol	1223.00		NIST Webbook
tb	485.07	K	Joback Method
tc	705.71	K	Joback Method
tf	319.82	K	Aqueous Solubility Prediction Method

vc	0.371	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	240.73	J/mol×K	668.94	Joback Method
cpg	194.52	J/mol×K	485.07	Joback Method
cpg	205.12	J/mol×K	521.84	Joback Method
cpg	215.02	J/mol×K	558.62	Joback Method
cpg	224.23	J/mol×K	595.39	Joback Method
cpg	232.79	J/mol×K	632.16	Joback Method
cpg	248.09	J/mol×K	705.71	Joback Method
hsubt	77.80	kJ/mol	308.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	439.20	K	1.90	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	2.08769e+01
Coeff. B	-6.73733e+03
Coeff. C	-8.46050e+01
Temperature range (K), min.	411.83
Temperature range (K), max.	517.44

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1379.mol
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C103708&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
hsubt:	Enthalpy of sublimation at a given temperature
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
pvap:	Vapor 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