2,6-Xylidine

Other names:	1-AMINO-2,6-DIMETHYLBENZENE
	2,6-Dimethylaniline
	2,6-Dimethylbenzenamine
	2,6-Dimethylphenylamine
	2,6-Xylylamine
	2-AMINO-M-XYLENE
	2-Amino-1,3-dimethylbenzene
	2-Amino-1,3-xylene
	Aniline, 2,6-dimethyl-
	Benzenamine, 2,6-dimethyl-
	NCI-C56188
	NSC 7098
	o-Xylidine
Inchi:	InChI=1S/C8H11N/c1-6-4-3-5-7(2)8(6)9/h3-5H,9H2,1-2H3
InchiKey:	UFFBMTHBGFGIHF-UHFFFAOYSA-N
Formula:	C8H11N
SMILES:	Cc1cccc(C)c1N
Mol. weight [g/mol]:	121.18
CAS:	87-62-7

Physical Properties

Property code	Value	Unit	Source
af	0.4710		KDB
affp	901.70	kJ/mol	NIST Webbook
basg	869.80	kJ/mol	NIST Webbook
gf	176.08	kJ/mol	Joback Method
hf	38.93	kJ/mol	Joback Method
hfus	14.94	kJ/mol	Joback Method
hvap	59.60 ± 0.30	kJ/mol	NIST Webbook
ie	7.50 ± 0.10	eV	NIST Webbook
ie	7.36	eV	NIST Webbook
ie	7.78 ± 0.05	eV	NIST Webbook
ie	7.33 ± 0.05	eV	NIST Webbook
ie	7.30 ± 0.02	eV	NIST Webbook
log10ws	-2.06		Crippen Method
logp	1.886		Crippen Method
mcvol	109.800	ml/mol	McGowan Method

pc	4200.00	kPa	KDB
rinpol	1136.26		NIST Webbook
rinpol	1130.00		NIST Webbook
rinpol	1168.19		NIST Webbook
rinpol	196.15		NIST Webbook
rinpol	1149.00		NIST Webbook
rinpol	196.15		NIST Webbook
rinpol	1130.00		NIST Webbook
rinpol	1131.00		NIST Webbook
rinpol	1168.19		NIST Webbook
rinpol	1135.52		NIST Webbook
rinpol	1157.00		NIST Webbook
rinpol	1137.15		NIST Webbook
rinpol	1136.34		NIST Webbook
rinpol	1137.93		NIST Webbook
rinpol	1143.41		NIST Webbook
rinpol	1179.00		NIST Webbook
rinpol	1140.70		NIST Webbook
rinpol	1136.20		NIST Webbook
rinpol	1167.00		NIST Webbook
rinpol	1149.00		NIST Webbook
rinpol	1134.00		NIST Webbook
rinpol	1143.00		NIST Webbook
rinpol	1143.00		NIST Webbook
rinpol	1173.00		NIST Webbook
rinpol	1157.00		NIST Webbook
rinpol	1146.00		NIST Webbook
ripol	1940.00		NIST Webbook
sl	251.35	J/mol×K	NIST Webbook
tb	488.00 ± 1.00	K	NIST Webbook
tb	491.05	K	KDB
tc	722.00	K	KDB
tf	284.40 ± 1.00	K	NIST Webbook
tf	284.16 ± 0.30	K	NIST Webbook
tf	284.60	K	NIST Webbook
tf	284.15	K	KDB
vc	0.405	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	228.80	J/mol×K	491.61	Joback Method
cpg	240.98	J/mol×K	529.22	Joback Method
cpg	252.48	J/mol×K	566.83	Joback Method
cpg	263.33	J/mol×K	604.43	Joback Method
cpg	273.54	J/mol×K	642.04	Joback Method
cpg	283.15	J/mol×K	679.65	Joback Method
cpg	292.16	J/mol×K	717.26	Joback Method
cpl	238.86	J/mol×K	298.15	NIST Webbook
hvapt	59.20 ± 0.30	kJ/mol	306.00	NIST Webbook
hvapt	48.50	kJ/mol	431.50	NIST Webbook
hvapt	50.70	kJ/mol	404.00	NIST Webbook
rhol	981.57	kg/m3	293.10	KDB

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	487.20	K	98.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.48251e+01
Coeff. B	-4.19647e+03
Coeff. C	-7.68560e+01
Temperature range (K), min.	365.52
Temperature range (K), max.	517.96

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	2.29985e+01
Coeff. B	-6.15563e+03
Coeff. C	-9.61781e-01
Coeff. D	4.39184e-07
Temperature range (K), min.	373.15

Temperature range (K), max.	491.15

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1307.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C87627&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1307
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

af:	Acentric Factor
affp:	Proton affinity
basg:	Gas basicity
cpg:	Ideal gas heat capacity
cpl:	Liquid phase 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
hvapt:	Enthalpy of vaporization at a given temperature
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
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sl:	Liquid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume