

Benzenamine, 2,5-dimethyl-

Other names:	1-Amino-2,5-dimethylbenzene 2,5-Dimethylaniline 2,5-Dimethylbenzenamine 2,5-Dimethylbenzeneamine 2,5-Dimethylphenylamine 2,5-Xylidine 2-Amino-1,4-dimethylbenzene 2-Amino-1,4-xylene 3-Amino-1,4-dimethylbenzene 5-Amino-1,4-dimethylbenzene 5-Methyl-o-toluidine 6-Methyl-m-toluidine Aniline, 2,5-dimethyl- NSC 7639 p-Xylidine
Inchi:	InChI=1S/C8H11N/c1-6-3-4-7(2)8(9)5-6/h3-5H,9H2,1-2H3
InchiKey:	VOWZNBNDMFLQGM-UHFFFAOYSA-N
Formula:	C8H11N
SMILES:	<chem>Cc1ccc(C)c(N)c1</chem>
Mol. weight [g/mol]:	121.18
CAS:	95-78-3

Physical Properties

Property code	Value	Unit	Source
gf	176.08	kJ/mol	Joback Method
hf	38.93	kJ/mol	Joback Method
hfus	14.94	kJ/mol	Joback Method
hvap	47.64	kJ/mol	Joback Method
ie	7.50 ± 0.10	eV	NIST Webbook
ie	7.78 ± 0.05	eV	NIST Webbook
ie	7.20	eV	NIST Webbook
log10ws	-2.06		Crippen Method
logp	1.886		Crippen Method
mcvol	109.800	ml/mol	McGowan Method
pc	3773.04	kPa	Joback Method
rinpol	1142.80		NIST Webbook
rinpol	1142.30		NIST Webbook

rinpol	1142.80		NIST Webbook
rinpol	1142.30		NIST Webbook
rinpol	196.94		NIST Webbook
rinpol	1171.00		NIST Webbook
rinpol	196.94		NIST Webbook
tb	487.20	K	NIST Webbook
tb	491.20	K	NIST Webbook
tc	717.26	K	Joback Method
tf	279.00 ± 1.00	K	NIST Webbook
tf	287.40 ± 1.00	K	NIST Webbook
vc	0.405	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	283.15	J/mol×K	679.65	Joback Method
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	292.16	J/mol×K	717.26	Joback Method
hfust	13.70	kJ/mol	279.00	NIST Webbook
hfust	13.70	kJ/mol	279.00	NIST Webbook
hvapt	61.70 ± 0.70	kJ/mol	317.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.44845e+01
Coeff. B	-4.09072e+03
Coeff. C	-7.65780e+01
Temperature range (K), min.	364.72
Temperature range (K), max.	522.53

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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=C95783&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
hfust:	Enthalpy of fusion at a given temperature
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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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