Acetamide, N-phenyl-

Other names:	ACETANILINE
	AN [Analgesic]
	Acetamidobenzene
	Acetanil
	Acetanilid
	Acetanilide
	Acetic acid anilide
	Acetoanilide
	Acetylaminobenzene
	Acetylaniline
	Aniline, N-acetyl-
	Antifebrin
	Benzenamine, N-acetyl-
	N-Acetylaminobenzene
	N-Acetylaniline
	N-Phenylacetamide
	N-phenylethanamide
	NSC 7636
	Phenalgene
	Phenalgin
	USAF EK-3
Inchi:	InChI=1S/C8H9NO/c1-7(10)9-8-5-3-2-4-6-8/h2-6H,1H3,(H,9,10)
InchiKey:	FZERHIULMFGESH-UHFFFAOYSA-N
Formula:	C8H9NO
SMILES:	CC(=O)Nc1ccccc1
Mol. weight [g/mol]:	135.16
CAS:	103-84-4

Physical Properties

Property code	Value	Unit	Source
chs	-4224.80 ± 1.00	kJ/mol	NIST Webbook
chs	-4224.88 ± 0.93	kJ/mol	NIST Webbook
gf	89.36	kJ/mol	Joback Method
hf	-31.03	kJ/mol	Joback Method
hfs	-209.50 ± 1.50	kJ/mol	NIST Webbook
hfs	-209.40 ± 1.00	kJ/mol	NIST Webbook

hfus	22.10	kJ/mol	Vaporization and Sublimation Enthalpies of Acetanilide and Several Derivatives by Correlation Gas Chromatography
hfus	21.44	kJ/mol	Solid liquid equilibria for binary mixtures of N-phenylacetamide with 4-aminoacetophenone, 3-hydroxyacetophenone and 4-hydroxyacetophenone
hvap	48.86	kJ/mol	Joback Method
ie	8.46 ± 0.05	eV	NIST Webbook
ie	8.30 ± 0.10	eV	NIST Webbook
ie	8.60	eV	NIST Webbook
ie	8.18 ± 0.03	eV	NIST Webbook
ie	8.39 ± 0.10	eV	NIST Webbook
ie	8.46	eV	NIST Webbook
log10ws	-1.40		Aqueous and cosolvent solubility data for drug-like organic compounds
log10ws	-1.23		Aqueous Solubility Prediction Method
log10ws	-1.33		Estimated Solubility Method
logp	1.645		Crippen Method
mcvol	111.370	ml/mol	McGowan Method
nfpaf	%!d(float64=1)		KDB
nfpah	%!d(float64=3)		KDB
pc	4010.84	kPa	Joback Method
rinpol	1362.00		NIST Webbook
rinpol	1362.00		NIST Webbook
rinpol	1358.00		NIST Webbook
rinpol	1362.00		NIST Webbook
tb	577.20	K	NIST Webbook
tb	578.15 ± 2.00	K	NIST Webbook
tc	735.85	K	Joback Method
tf	387.47	K	Aqueous Solubility Prediction Method
tf	387.50	K	The use of organic calibration standards in the enthalpy calibration of differential scanning calorimeters
tt	387.52 ± 0.01	K	NIST Webbook
vc	0.416	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	278.21	J/mol×K	661.62	Joback Method
cpg	287.28	J/mol×K	698.74	Joback Method
cpg	234.64	J/mol×K	513.16	Joback Method
cpg	246.69	J/mol×K	550.28	Joback Method
cpg	257.95	J/mol×K	587.39	Joback Method
cpg	268.45	J/mol×K	624.51	Joback Method
cpg	295.69	J/mol×K	735.85	Joback Method
cps	179.30	J/mol×K	298.15	NIST Webbook
cps	191.60	J/mol×K	323.00	NIST Webbook
hfust	21.67	kJ/mol	387.50	NIST Webbook
hfust	21.65	kJ/mol	387.50	NIST Webbook
hfust	21.40	kJ/mol	386.90	NIST Webbook
hfust	18.30	kJ/mol	387.20	NIST Webbook
hsubt	87.20	kJ/mol	326.50	NIST Webbook
hsubt	80.60	kJ/mol	313.50	NIST Webbook
hvapt	66.30	kJ/mol	482.00	NIST Webbook
hvapt	64.80	kJ/mol	525.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	2.21222e+01
Coeff. B	-7.49417e+03
Coeff. C	-9.38710e+01
Temperature range (K), min.	437.09
Temperature range (K), max.	539.67

Sources

Vaporization and Sublimation Enthalpies of Acetanilide and Several Derivatives by Correlation Gas Chromatography:	https://www.doi.org/10.1021/je300152t
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
The use of organic calibration standards in the enthalpy calibration of differential scanning calorimeters:	https://www.doi.org/10.1016/j.tca.2012.03.028
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C103844&Units=SI
Experimental Measurements and Correlation of the Solubility of Three Primary Amides in Supercritical CO2:	https://www.doi.org/10.1021/je400357t
Aqueous and cosolvent solubility data for drug-like organic compounds:	https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Butanamide:	
Calibration and test of an aneroid mini-bomb combustion calorimeter:	https://www.doi.org/10.1016/j.jct.2006.10.013
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1380
Partial molar volumes of some drug and pro-drug substances in 1-octanol at T = 298.15 K:	https://www.doi.org/10.1016/j.jct.2009.10.002
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Solid liquid equilibria for binary mixtures of N-phenylacetamide with 4-aminoacetophenone, 3-hydroxyacetophenone and 4-hydroxyacetophenone:	https://www.doi.org/10.1016/j.fluid.2005.03.023

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsubt:	Enthalpy of sublimation 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
nfpaf:	NFPA Fire Rating
nfpah:	NFPA Health Rating
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume