Acetaminophen

Other names:

4'-Hydroxyacetanilide
4-(Acetylamino)phenol
4-(N-Acetylamino)phenol
4-Acetamidophenol
4-Acetaminophenol
4-Hydroxyacetanilide
4-Hydroxyanilid kyseliny octove
APAP
Abensanil
Acamol
Accu-Tap
Acenol
Acetagesic
Acetalgin
Acetamide, N-(4-hydroxyphenyl)-
Acetamide, N-(p-hydroxyphenyl)-
Acetaminofen
Acetanilide, 4'-hydroxy-
Algotropyl
Alpiny
Alpinyl
Alvedon
Amadil
Anaflon
Anapap
Anelix
Anhiba
Apadon
Apamid
Apamide
Banesin
Ben-u-Ron
Bickie-mol
Biocetamol
Calpol
Captin
Cetadol
Citramon P
Claratal
Clixodyne

Cyclopam
Dafalgan
Daga
Daphalgan
Datril
Dial-a-gesic
Dimindol
Dirox
Disprol
Doliprane
Dolprone
Dularin
Dymadon
Dypap
Elixodyne
Enelfa
Eneril
Eu-Med
Exdol
Febridol
Febrilix
Febrinol
Febro-Gesic
Febrolin
Fendon
Finimal
G 1
Gelocatil
Hedex
Homoolan
Injectapap
Janupap
Korum
Lestemp
Liquagesic
Lonarid
Lyteca
Lyteca Syrup
Minoset
Momentum
Multin
N-(4-Hydroxyphenyl)acetamide
N-(4-hydroxyphenyl)ethanamide

N-(p-Hydroxyphenyl) acetamide
N-Acetyl-4-aminophenol
N-Acetyl-4-hydroxyaniline
N-Acetyl-p-aminophenol
NAPA
NAPAP
NCI-C55801
Napafen
Naprinol
Nealgyl
Nebs
Neotrend
Nobedon
Ortensan
Pacemo
Pacemol
Painex
Paldesic
Panadol
Panaleve
Panasorb
Panets
Panex
Panodil
Panofen
Paracet
Paracetamol
Paracetamol DC
Paracetamole
Paracetamolo
Paracetanol
Parapan
Paraspen
Parelan
Parmol
Pasolind N
Pedric
Phenaphen
Phendon
Phenol, p-acetamido-
Pinex
Pyral
Pyrinazine

	Resfenol
	Resprin
	Rivalgyl
	SK-Apap
	Salzone
	Servigesic
	St. Joseph Fever Reducer
	Tabalgin
	Tapar
	Temlo
	Tempanal
	Tempra
	Tralgon
	Tussapap
	Tylenol
	Valadol
	Valgesic
	Vermidon
	p-(Acetylamino)phenol
	p-Acetamidophenol
	p-Acetoaminophen
	p-Hydroxyacetanilide
	p-Hydroxyphenolacetamide
Inchi:	InChI=1S/C8H9NO2/c1-6(10)9-7-2-4-8(11)5-3-7/h2-5,11H,1H3,(H,9,10)
InchiKey:	RZVAJINKPMORJF-UHFFFAOYSA-N
Formula:	C8H9NO2
SMILES:	CC(=O)Nc1ccc(O)cc1
Mol. weight [g/mol]:	151.16
CAS:	103-90-2

Physical Properties

Property code	Value	Unit	Source
gf	-65.26	kJ/mol	Joback Method
hf	-208.34	kJ/mol	Joback Method
hfus	24.90	kJ/mol	Study of Glass Transition Phenomena in the Supercooled Liquid Phase of Methocarbamol, Acetaminophen and Mephensin
hsub	138.00 ± 3.00	kJ/mol	NIST Webbook

hvap	61.87	kJ/mol	Joback Method
ie	7.57 ± 0.02	eV	NIST Webbook
log10ws	-1.06		Aqueous Solubility Prediction Method
log10ws	-1.07		Aqueous and cosolvent solubility data for drug-like organic compounds
log10ws	-1.03		Estimated Solubility Method
logp	1.351		Crippen Method
mcvol	117.240	ml/mol	McGowan Method
pc	4890.21	kPa	Joback Method
rinpol	1643.00		NIST Webbook
rinpol	1632.00		NIST Webbook
rinpol	1631.00		NIST Webbook
rinpol	1694.00		NIST Webbook
rinpol	1631.00		NIST Webbook
rinpol	1636.00		NIST Webbook
rinpol	1703.00		NIST Webbook
rinpol	1697.00		NIST Webbook
rinpol	1636.00		NIST Webbook
rinpol	1687.00		NIST Webbook
rinpol	1668.00		NIST Webbook
rinpol	1678.00		NIST Webbook
rinpol	1664.00		NIST Webbook
rinpol	1650.00		NIST Webbook
rinpol	1668.00		NIST Webbook
rinpol	1631.00		NIST Webbook
tb	593.78	K	Joback Method
tc	827.84	K	Joback Method
tf	441.85	K	DSC study and phase diagrams calculation of binary systems of paracetamol
tf	445.60	K	Vapor pressures and standard molar enthalpies, entropies and Gibbs energies of sublimation of three 4-substituted acetanilide derivatives
tf	442.35	K	Determination and prediction of solubilities of active pharmaceutical ingredients in selected organic solvents
tf	442.15	K	Liquid pharmaceuticals formulation by eutectic formation

tf	443.15	K	Solubility of Anti-Inflammatory, Anti-Cancer, and Anti-HIV Drugs in Supercritical Carbon Dioxide
tf	441.20 ± 0.50	K	NIST Webbook
tf	441.00 ± 2.00	K	NIST Webbook
tt	297.00	K	Endothermic features on heating of glasses show that the second glass to liquid transition of water was phenomenologically-mistaken
vc	0.383	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	325.46	J/mol×K	788.83	Joback Method
cpg	332.79	J/mol×K	827.84	Joback Method
cpg	280.17	J/mol×K	593.78	Joback Method
cpg	290.67	J/mol×K	632.79	Joback Method
cpg	300.36	J/mol×K	671.80	Joback Method
cpg	309.33	J/mol×K	710.81	Joback Method
cpg	317.67	J/mol×K	749.82	Joback Method
hfust	26.02	kJ/mol	441.20	NIST Webbook
hfust	26.20	kJ/mol	443.00	NIST Webbook
hfust	27.60	kJ/mol	443.20	NIST Webbook
hfust	27.00	kJ/mol	440.30	NIST Webbook
hfust	26.49	kJ/mol	441.90	NIST Webbook
hvapt	99.00 ± 1.00	kJ/mol	494.00	NIST Webbook
hvapt	103.00 ± 3.00	kJ/mol	521.00	NIST Webbook

Sources

Partial molar volume of paracetamol in water, 0.1 M HCl and 0.154 M NaCl at T = (298.15, 303.15, 308.15 and 310.65) K and at 101.325 kPa: https://www.doi.org/10.1016/j.jct.2005.03.008

Aqueous solubility of acetaminophen in the presence of 1-hexyl-3- methyl imidazolium bromide, ionic liquid as co-solvent: https://www.doi.org/10.1016/j.fluid.2016.05.012

Dynamic and Static Characteristics of Drug Dissolution in Supercritical CO2 by Infrared Spectroscopy: https://www.doi.org/10.1021/je500456s

Solubility of Anti-Inflammatory, Anti-Cancer, and Anti-HIV Drugs in Supercritical Carbon Dioxide: https://www.doi.org/10.1021/je049551l

Measurements of Acetaminophen Solubility in a Wide Range of State Parameters:

Experimental and Modeling Studies on the Solubility of 2-Chloro-N-(4-methylphenyl)propanamide (S1) in Binary Ethyl Acetate + Hexane, Toluene + Hexane, Acetone + Hexane, and Butanone + Hexane Solvent Mixtures Using Polythermal Method: https://www.doi.org/10.1021/acs.jced.7b00288

Solid-Liquid Phase Equilibrium of N,N'-Piperazinebis(neopentylglycol)phosphoramidate in Selected Solvents from T = (292.15 to 333.15) K: https://www.doi.org/10.1021/acs.jced.7b00206

Endothermic features on heating of glasses show that the second glass to liquid transition of water was phenomenologically-mistaken:	https://www.doi.org/10.1016/j.tca.2016.11.011
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
DSC study and phase diagrams calculation of binary systems of paracetamol:	https://www.doi.org/10.1016/j.tca.2012.09.024
Solubilization Behavior of Paracetamol in Transcutol Water Mixtures at (298.15 to 333.15) K:	https://www.doi.org/10.1021/je4008525
Vapor pressures and standard molar enthalpies, entropies and Gibbs energies of sublimation of three 4-substituted acetanilide derivatives:	https://www.doi.org/10.1016/j.fluid.2009.02.001
Study of Glass Transition Phenomena in the Supercooled Liquid Phase of Methocarbamol, Acetaminophen and Ibuprofen:	https://www.doi.org/10.1016/j.tca.2013.10.035
Determination and prediction of solubilities of active pharmaceutical ingredients in selected organic solvents:	https://www.doi.org/10.1016/j.fluid.2015.07.032
Solubility Measurement and Thermodynamic Modeling of Liquid Pharmaceuticals formulation by eutectic formation:	https://www.doi.org/10.1021/acs.jced.7b01011
N-(4-Methylphenyl)-2-chloro-2-(phenylthio)propenamide in 12 Pure Solvents at Temperatures Ranging from 278.15 to 318.15 K:	https://www.doi.org/10.1016/j.fluid.2017.05.009
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
Effect of paracetamol in aqueous sodium malonate solutions with reference to volumetric and viscometric measurements:	https://www.doi.org/10.1016/j.jct.2015.12.024
Solubilities of Pharmaceutical Compounds in Ionic Liquids :	https://www.doi.org/10.1021/je101040p
Effect of Some Imidazolium-Based Ionic Liquids with Different Anions on the Thermodynamic Properties of Acetaminophen in Aqueous Media at T = 293.15 to 308.15 K:	https://www.doi.org/10.1021/acs.jced.7b00464
Gripper Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Activity coefficients of the species in the methanol solutions of acetaminophen and two silylated derivatives at 298.15K:	https://www.doi.org/10.1016/j.fluid.2006.08.020
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C103902&Units=SI
Pressurized-Synthetic Methodology for Solubility Determination at Elevated Temperatures With Application to Paracetamol in Pure Solvents:	https://www.doi.org/10.1021/acs.jced.7b00118
Diffusion coefficients of paracetamol in aqueous solutions:	https://www.doi.org/10.1016/j.jct.2012.03.014
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Experimental determination and correlation of acetaminophen solubility in aqueous solutions of choline chloride-based deep eutectic solvents and	https://www.doi.org/10.1016/j.fluid.2018.01.017
Measurement and Correlation of Solubility of Resorcinol Bis(cyclic 2,2-dimethyl-1,3-propanediol phosphate) in Selected Solvents from T = 293.15 to 333.15 K:	https://www.doi.org/10.1021/acs.jced.7b00695

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
hsub:	Enthalpy of sublimation 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
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