Phenacetin

Other names:

1-Acetamido-4-ethoxybenzene
4'-Ethoxyacetanilide
4-(Acetylamino)phenetole
4-Ethoxy-acetanilid
4-Ethoxyacetanilide
APC
ASA COMPOUND
Acet-p-phenalide
Acet-p-phenetidin
Acetamide, N-(4-ethoxyphenyl)-
Acetanilide, 4'-ethoxy-
Acetanilide, p-ethoxy-
Aceto-4-phenetidine
Aceto-para-phenalide
Aceto-para-phenetidide
Acetophenetidin
Acetophenetidine
Acetophenetin
Acetphenetidin
Acetylphenetidin
Achrocidin
Anapac
Bromo seltzer
Buff-A-comp
Citra-fort
Clistanol
Codempiral
Commotional
Contradol
Contradouleur
Coricidin
Coriforte
Coryban-D
Daprisal
Darvon compound
Dasikon
Dasin
Dasin CH
Dolostop
Dolviran

Edrisal
Empiral
Empirin compound
Emprazil
Emprazil-C
Epragen
Fenacetin
Fenacetina
Fenia
Fenidina
Fenina
Fiorinal
Fortacyl
Gelonida
Gewodin
Helvagit
Hjorton'S powder
Hocophen
KAFA
Kalmin
Malex
Melabon
Melaforte
N-(4-Ethoxyphenyl)acetamide
N-(4-ethoxyphenyl)ethanamide
N-Acetyl-4-ethoxyaniline
N-Acetyl-p-ethoxyaniline
N-Acetyl-p-phenetidine
N-para-Ethoxyphenylacetamide
Norgesic
Pamprin
Para-acetphenetidin
Paracetophenetidin
Paramette
Paratodol
Pertonal
Phenacet
Phenacetine
Phenacetinum
Phenacitin
Phenacon
Phenaphen
Phenaphen plus

Phenazetin
Phenazetina
Phenedina
Phenidin
Phenin
Phenodyne
Pyraphen
Pyrroxate
Quadronal
RCRA Waste number U187
Robaxisal-PH
Salgydal
Sanalgine
Saridon
Seranex
Sinedal
Sinubid
Sinutab
Stellacyl
Super anahist
Synalgos-DC
Synalogos
Tacol
Terracydin
Tetracydin
Thephorin A-C
Treupel
Veganine
Viden
Wigraine
Xaril
Zactirin compound
ethanamide, N-(4-ethoxyphenyl)-
p-Acetophenetide
p-Acetophenetidide
p-Acetophenetidine
p-Acetophenetitide
p-Acetphenetidin
p-Ethoxyacetanilide
p-Ethoxyanilid kyseliny octove
p-Phenetidine, N-acetyl-
p-phenacetin
para-Acetophenetidide

	para-Phenacetin
Inchi:	InChI=1S/C10H13NO2/c1-3-13-10-6-4-9(5-7-10)11-8(2)12/h4-7H,3H2,1-2H3,(H,11,12)
InchiKey:	CPJSUEIXXCENMM-UHFFFAOYSA-N
Formula:	C10H13NO2
SMILES:	CCOc1ccc(N=C(C)O)cc1
Mol. weight [g/mol]:	179.22
CAS:	62-44-2

Physical Properties

Property code	Value	Unit	Source
chs	-5452.00	kJ/mol	NIST Webbook
hf	-236.69	kJ/mol	Joback Method
hfs	-341.00	kJ/mol	NIST Webbook
hfus	32.00	kJ/mol	Vaporization and Sublimation Enthalpies of Acetanilide and Several Derivatives by Correlation Gas Chromatography
hsub	120.00 ± 3.00	kJ/mol	NIST Webbook
hsub	115.00	kJ/mol	NIST Webbook
hvap	63.28	kJ/mol	Joback Method
log10ws	-2.32		Aqueous Solubility Prediction Method
log10ws	-2.35		Estimated Solubility Method
logp	2.693		Crippen Method
mcvol	145.420	ml/mol	McGowan Method
pc	2808.38	kPa	Joback Method
rinpol	1660.00		NIST Webbook
rinpol	1666.00		NIST Webbook
rinpol	1681.00		NIST Webbook
rinpol	1720.00		NIST Webbook
rinpol	1700.00		NIST Webbook
rinpol	1675.00		NIST Webbook
rinpol	1685.00		NIST Webbook
rinpol	1660.00		NIST Webbook
rinpol	1685.00		NIST Webbook
rinpol	1660.00		NIST Webbook
rinpol	1651.00		NIST Webbook
rinpol	1662.00		NIST Webbook
rinpol	1681.00		NIST Webbook
rinpol	1690.00		NIST Webbook

rinpol	1705.00		NIST Webbook
rinpol	1651.00		NIST Webbook
rinpol	1660.00		NIST Webbook
rinpol	1699.00		NIST Webbook
rinpol	1685.00		NIST Webbook
rinpol	1668.00		NIST Webbook
rinpol	1660.00		NIST Webbook
rinpol	285.77		NIST Webbook
rinpol	288.72		NIST Webbook
rinpol	1705.00		NIST Webbook
rinpol	285.77		NIST Webbook
rinpol	1662.00		NIST Webbook
rinpol	1660.00		NIST Webbook
rinpol	1670.00		NIST Webbook
rinpol	1681.00		NIST Webbook
rinpol	1681.00		NIST Webbook
rinpol	1670.00		NIST Webbook
rinpol	1680.00		NIST Webbook
rinpol	1666.00		NIST Webbook
rinpol	1660.00		NIST Webbook
rinpol	1651.00		NIST Webbook
rinpol	1700.00		NIST Webbook
rinpol	1685.00		NIST Webbook
rinpol	1695.00		NIST Webbook
rinpol	1699.00		NIST Webbook
rinpol	1675.00		NIST Webbook
tb	651.02	K	Joback Method
tc	860.75	K	Joback Method
tf	410.00 ± 1.00	K	NIST Webbook
tf	409.60	K	Vapor pressures and standard molar enthalpies, entropies and Gibbs energies of sublimation of three 4-substituted acetanilide derivatives
tf	408.53	K	Aqueous Solubility Prediction Method
tf	407.20 ± 0.50	K	NIST Webbook
tf	410.00 ± 0.60	K	NIST Webbook
tt	407.00	K	Solubility of n-(4-Ethoxyphenyl)ethanamide in Supercritical Carbon Dioxide

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	34.10	kJ/mol	407.40	NIST Webbook
hfust	21.40	kJ/mol	410.20	NIST Webbook
hfust	31.25	kJ/mol	407.20	NIST Webbook
hfust	28.75	kJ/mol	408.30	NIST Webbook
hfust	30.00	kJ/mol	409.60	NIST Webbook
hsubt	115.50 ± 2.40	kJ/mol	349.50	NIST Webbook
hvapt	82.60	kJ/mol	498.00	NIST Webbook
hvapt	79.00 ± 1.00	kJ/mol	459.00	NIST Webbook
hvapt	82.00 ± 1.00	kJ/mol	476.00	NIST Webbook

Sources

Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Solubility of Phenacetinum in Methanol, Ethanol, 1-Propanol, 1-Butanol, 1-Pentanol, Tetrahydrofuran, Ethyl Acetate, and Benzene between 282.65 K and 333.70 K:	https://www.doi.org/10.1021/je700209v
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C62442&Units=SI
Solubility of n-(4-Ethoxyphenyl)ethanamide in Supercritical Carbon Dioxide:	https://www.doi.org/10.1021/je900614f
Vaporization and Sublimation Enthalpies of Acetanilide and Several Derivatives by Correlation Gas Chromatography:	https://www.doi.org/10.1021/je300152t
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
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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chs:	Standard solid enthalpy of combustion
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
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature

hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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