Benzamide, 2-hydroxy-

Other names:

2-Carbamoylphenol
2-Carboxamidophenol
2-hydroxybenzamide
Acket
Afko-Sal
Algamon
Algiamida
Allevin
Amid kyseliny salicylove
Amid-Sal
Amidosal
Anamid
Andasol
Benesal
Benzamide, o-hydroxy-
Cetamide
Cidal
Cymidon
Dolomide
Dropsprin
Eggosalil
Flarpirina
H.P. 34
Liquiprin
Morsarinas
NSC 3115
Novecyl
OHB
Oramid
Panithal
Raspberin
SR 4326
Salamid
Salamide
Saliamid
Saliamin
Salicilamide
Salicim
Salicylamid
Salicylic Acid amide

Salipur
Salizell
Salrin
Salymid
Samid
Serramida
Urtosal
o-hydroxybenzamide
salicylamide

Inchi: InChI=1S/C7H7NO2/c8-7(10)5-3-1-2-4-6(5)9/h1-4,9H,(H2,8,10)
InchiKey: SKZKKFZAGNVIMN-UHFFFAOYSA-N
Formula: C7H7NO2
SMILES: NC(=O)c1ccccc1O
Mol. weight [g/mol]: 137.14

Physical Properties

Property code	Value	Unit	Source
af	0.6758		Cheméo Relay (1.0)
chs	-3352.40 ± 2.20	kJ/mol	NIST Webbook
gf	-96.62	kJ/mol	Joback Method
hf	-330.45	kJ/mol	Cheméo Relay (1.0)
hfs	-402.70 ± 2.20	kJ/mol	NIST Webbook
hfus	27.40	kJ/mol	Thermodynamic and structural aspects of hydroxybenzamide molecular crystals study
hfus	29.00	kJ/mol	Solubility and Melting Properties of Salicylamide
hsub	99.30 ± 1.30	kJ/mol	NIST Webbook
hsub	101.90 ± 0.40	kJ/mol	NIST Webbook
hvap	66.30	kJ/mol	Cheméo Relay (1.0)
ie	8.58	eV	Cheméo Relay (1.0)
log10ws	-1.78		Aqueous Solubility Prediction Method
log10ws	-1.82		Estimated Solubility Method
logp	0.491		Crippen Method
mcvol	103.150	ml/mol	McGowan Method
pc	6009.25	kPa	Joback Method
rinpol	1399.00		NIST Webbook
rinpol	1435.00		NIST Webbook
rinpol	1422.00		NIST Webbook

rinpol	1450.00		NIST Webbook
rinpol	1445.00		NIST Webbook
rinpol	1450.00		NIST Webbook
rinpol	1450.00		NIST Webbook
rinpol	1460.00		NIST Webbook
rinpol	1470.00		NIST Webbook
rinpol	1450.00		NIST Webbook
rinpol	1450.00		NIST Webbook
rinpol	1405.00		NIST Webbook
rinpol	1405.00		NIST Webbook
rinpol	1397.00		NIST Webbook
rinpol	1402.00		NIST Webbook
rinpol	1409.00		NIST Webbook
rinpol	1435.00		NIST Webbook
rinpol	1435.00		NIST Webbook
rinpol	1455.00		NIST Webbook
rinpol	1405.00		NIST Webbook
rinpol	1399.00		NIST Webbook
tb	543.50	K	Cheméo Relay (1.0)
tc	825.12	K	Cheméo Relay (1.0)
tf	414.00 ± 1.00	K	NIST Webbook
tf	413.95	K	Aqueous Solubility Prediction Method
vc	0.356	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	242.37	J/mol×K	593.26	Joback Method
cpg	287.34	J/mol×K	841.84	Joback Method
cpg	281.13	J/mol×K	800.41	Joback Method
cpg	274.53	J/mol×K	758.98	Joback Method
cpg	267.46	J/mol×K	717.55	Joback Method
cpg	259.81	J/mol×K	676.12	Joback Method
cpg	251.48	J/mol×K	634.69	Joback Method
cps	163.30	J/mol×K	360.40	Determination of the activity of a molecular solute in saturated solution

cps	172.90	J/mol×K	380.40	Determination of the activity of a molecular solute in saturated solution
cps	145.50	J/mol×K	325.40	Determination of the activity of a molecular solute in saturated solution
cps	148.10	J/mol×K	330.40	Determination of the activity of a molecular solute in saturated solution
cps	150.50	J/mol×K	335.40	Determination of the activity of a molecular solute in saturated solution
cps	153.10	J/mol×K	340.40	Determination of the activity of a molecular solute in saturated solution
cps	155.60	J/mol×K	345.40	Determination of the activity of a molecular solute in saturated solution
cps	158.20	J/mol×K	350.40	Determination of the activity of a molecular solute in saturated solution
cps	160.60	J/mol×K	355.40	Determination of the activity of a molecular solute in saturated solution
cps	124.10	J/mol×K	280.40	Determination of the activity of a molecular solute in saturated solution
cps	165.60	J/mol×K	365.40	Determination of the activity of a molecular solute in saturated solution
cps	168.10	J/mol×K	370.40	Determination of the activity of a molecular solute in saturated solution
cps	170.30	J/mol×K	375.40	Determination of the activity of a molecular solute in saturated solution

cps	142.90	J/mol×K	320.40	Determination of the activity of a molecular solute in saturated solution
cps	175.40	J/mol×K	385.40	Determination of the activity of a molecular solute in saturated solution
cps	177.90	J/mol×K	390.40	Determination of the activity of a molecular solute in saturated solution
cps	180.60	J/mol×K	395.40	Determination of the activity of a molecular solute in saturated solution
cps	126.30	J/mol×K	285.40	Determination of the activity of a molecular solute in saturated solution
cps	128.70	J/mol×K	290.40	Determination of the activity of a molecular solute in saturated solution
cps	140.50	J/mol×K	315.40	Determination of the activity of a molecular solute in saturated solution
cps	138.00	J/mol×K	310.40	Determination of the activity of a molecular solute in saturated solution
cps	135.60	J/mol×K	305.40	Determination of the activity of a molecular solute in saturated solution
cps	133.10	J/mol×K	300.40	Determination of the activity of a molecular solute in saturated solution
cps	130.90	J/mol×K	295.40	Determination of the activity of a molecular solute in saturated solution
hfust	29.00	kJ/mol	411.90	NIST Webbook
hfust	27.10	kJ/mol	414.90	NIST Webbook

hvapt	113.70	kJ/mol	298.15	Thermochemical studies on salicylaldehyde and salicylamide

Sources

Determination of the activity of a molecular solute in saturated solution:	https://www.doi.org/10.1016/j.jct.2008.06.016
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Effect of temperature on volumetric and viscometric properties of some non-steroidal anti-inflammatory drugs in aprotic solvents:	https://www.doi.org/10.1016/j.jct.2010.03.009
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C65452&Units=SI
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
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Cheméo Relay (1.0):	
Volumetric and Viscometric Studies of Salicyl Amide, Salicylic Acid, and Acetyl Salicylic Acid in Alcohols at Different Temperatures:	https://www.doi.org/10.1021/je800616p
Cheméo Relay (1.0, beta):	
Solubility and Melting Properties of Salicylamide:	https://www.doi.org/10.1021/je060178m
Thermochemical studies on salicylaldehyde and salicylamide:	https://www.doi.org/10.1016/j.jct.2007.03.006
Thermodynamic and structural aspects of hydroxybenzamide molecular crystals study:	https://www.doi.org/10.1016/j.tca.2012.10.013
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

Legend

af:	Acentric Factor
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
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
vc:	Critical Volume