

Salicylamide

Other names: 2-Carbamoylphenol
2-Carboxamidophenol
2-Hydroxybenzamide
Acket
Afko-Sal
Algamon
Algiamida
Allevin
Amid kyseliny salicylove
Amid-Sal
Amidosal
Anamid
Andasol
Benesal
Benzamide, 2-hydroxy-
Benzamide, o-hydroxy-
Cetamide
Cidal
Cymidon
Dolomite
Dropsprin
Eggosalil
Flarpirina
H.P. 34
Liquiprin
Morsarinás
NSC 3115
Novecyl
OHB
Oramid
Panithal
Raspberin
SR 4326
Salamid
Salamide
Sali amid
Sali amine
Salicilamide
Salicim
Salicylamid

Salicylic Acid amide

Salipur

Salizell

Salrin

Salymid

Samid

Serramida

Urtosal

o-Hydroxybenzamide

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

CAS: 65-45-2

Physical Properties

Property code	Value	Unit	Source
chs	-3352.40 ± 2.20	kJ/mol	NIST Webbook
gf	-96.62	kJ/mol	Joback Method
hf	-207.38	kJ/mol	Joback Method
hfs	-402.70 ± 2.20	kJ/mol	NIST Webbook
hfus	29.00	kJ/mol	Solubility and Melting Properties of Salicylamide
hfus	27.40	kJ/mol	Thermodynamic and structural aspects of hydroxybenzamide molecular crystals study
hsub	101.90 ± 0.40	kJ/mol	NIST Webbook
hsub	99.30 ± 1.30	kJ/mol	NIST Webbook
hvap	63.85	kJ/mol	Joback Method
log10ws	-1.82		Estimated Solubility Method
log10ws	-1.78		Aqueous Solubility Prediction Method
logp	0.491		Crippen Method
mcvol	103.150	ml/mol	McGowan Method
pc	6009.25	kPa	Joback Method
rinpol	1402.00		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	1422.00		NIST Webbook
rinpol	1450.00		NIST Webbook
rinpol	1405.00		NIST Webbook
rinpol	1405.00		NIST Webbook
rinpol	1435.00		NIST Webbook
rinpol	1399.00		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
rinpol	1397.00		NIST Webbook
rinpol	1450.00		NIST Webbook
rinpol	1450.00		NIST Webbook
tb	593.26	K	Joback Method
tc	841.84	K	Joback Method
tf	413.95	K	Aqueous Solubility Prediction Method
tf	414.00 ± 1.00	K	NIST Webbook
vc	0.321	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	281.13	J/mol×K	800.41	Joback Method
cpg	287.34	J/mol×K	841.84	Joback Method
cpg	242.37	J/mol×K	593.26	Joback Method
cpg	251.48	J/mol×K	634.69	Joback Method
cpg	259.81	J/mol×K	676.12	Joback Method
cpg	267.46	J/mol×K	717.55	Joback Method
cpg	274.53	J/mol×K	758.98	Joback Method
cps	180.60	J/mol×K	395.40	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	124.10	J/mol×K	280.40	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	130.90	J/mol×K	295.40	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	135.60	J/mol×K	305.40	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	140.50	J/mol×K	315.40	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	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	163.30	J/mol×K	360.40	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	172.90	J/mol×K	380.40	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
hfust	29.00	kJ/mol	411.90	NIST Webbook
hfust	27.10	kJ/mol	414.90	NIST Webbook

Sources

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
Solubility and Melting Properties of Salicylamide:	https://www.doi.org/10.1021/je060178m
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Determination of the activity of a molecular solute in saturated solution:	https://www.doi.org/10.1016/j.jct.2008.06.016
Effect of temperature on volumetric and viscometric properties of some N-hydroxyamides:	https://www.doi.org/10.1016/j.jct.2010.03.009
Numerical and Statistical Studies of Salicylamide, Salicylic Acid, and Acetyl Salicylic Acid and Structural Aspects of Different Benzamide Molecular Crystals	https://www.doi.org/10.1021/je800616p
Different Benzamide molecular crystals study	https://www.doi.org/10.1016/j.tca.2012.10.013
Water Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C65452&Units=SI
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

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
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

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