

Salicylanilide

Other names:

2-Hydroxy-N-phenylbenzamide
2-Hydroxybenzanilide
ASK
Anilid kyseliny salicylove
Ansadol
Aseptolan
Benzamide, 2-hydroxy-N-phenyl-
Hyanilid
N-Phenylsalicylamide
NSC 14881
Salicylanilid
Salicylic acid anilide
Salifebrin
Salinide
Salinidol
Salnide
Sherstat SLN
Shirlan
Shirlan AG
Shirlan Extra
WR 10019
o-Hydroxybenzanilide

Inchi:

InChI=1S/C13H11NO2/c15-12-9-5-4-8-11(12)13(16)14-10-6-2-1-3-7-10/h1-9,15H,(H,14,16)O

InchiKey:

WKEDVNSFRWHDNR-UHFFFAOYSA-N

Formula:

C13H11NO2

SMILES:

O=C(Nc1ccccc1)c1ccccc1O

Mol. weight [g/mol]:

213.23

CAS:

87-17-2

Physical Properties

Property code	Value	Unit	Source
chs	-6379.60 ± 3.00	kJ/mol	NIST Webbook
gf	89.25	kJ/mol	Joback Method
hf	-75.01	kJ/mol	Joback Method
hfs	-308.20 ± 3.00	kJ/mol	NIST Webbook
hfus	29.99	kJ/mol	Joback Method

hvap	75.28		kJ/mol	Joback Method
log10ws	-3.59			Estimated Solubility Method
log10ws	-3.59			Aqueous Solubility Prediction Method
logp	2.644			Crippen Method
mcvol	163.930		ml/mol	McGowan Method
pc	4010.84		kPa	Joback Method
tb	734.86		K	Joback Method
tc	990.96		K	Joback Method
tf	409.90		K	Aqueous Solubility Prediction Method
vc	0.554		m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	437.15	J/mol×K	734.86	Joback Method
cpg	449.43	J/mol×K	777.54	Joback Method
cpg	460.74	J/mol×K	820.23	Joback Method
cpg	471.24	J/mol×K	862.91	Joback Method
cpg	481.08	J/mol×K	905.59	Joback Method
cpg	490.42	J/mol×K	948.27	Joback Method
cpg	499.42	J/mol×K	990.96	Joback Method

Sources

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C87172&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Joback Method:

https://en.wikipedia.org/wiki/Joback_method

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

Legend

chs: Standard solid enthalpy of combustion

cpg:	Ideal gas 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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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