Phenol, 2,2'-[1,2-ethanediylbis(nitrilomethylidyne)]bis-

Other names: 1,2-Bis(salicylidenamino)ethane
1,2-Ethanediamine, N,N'-bis[(2-hydroxyphenyl)methylene]-
2,2'-((ethane-1,2-diylbis(azanylylidene))bis(methanylylidene))diphenol
2,2'-[ethylenebis(nitrilomethylidyne)]diphenol
Bis(salicylaldehyde)ethylenediamine
Disalicylalethylenediamine
Disalicylidene-1,2-ethanediamine
Ethylene bis(salicylimine)
Ethylenediamine, N,N'-disalicylidene-
N,N'-Bis(salicylidene)ethylenediamine
N,N'-Disalicylideneethylenediamine
N,N'-Ethylene diimino di(o-cresol)
N,N'-Ethylenebis(salicylideneimine)
N,N'-bis(2-hydroxybenzylidene)-1,2-ethanediamine
NSC 2079
Salen
USAF DO-63
alpha,alpha'-(Ethylenedinitrilo)di-o-cresol
o-Cresol, «alpha»,«alpha»'-(ethylenedinitrilo)di-
«alpha»,«alpha»'-(Ethylenedinitrilo)di-o-cresol

Inchi: InChI=1S/C16H16N2O2/c19-15-7-3-1-5-13(15)11-17-9-10-18-12-14-6-2-4-8-16(14)20/h1

InchiKey: VEUMANXWQDHAJV-UHFFFAOYSA-N

Formula: C16H16N2O2

SMILES: Oc1ccccc1C=NCCN=Cc1ccccc1O

Mol. weight [g/mol]: 268.31

CAS: 94-93-9

Physical Properties

Property code	Value	Unit	Source
hf	-90.69	kJ/mol	Joback Method
hsub	141.30 ± 3.20	kJ/mol	NIST Webbook
hvap	88.42	kJ/mol	Joback Method
ie	8.53 ± 0.07	eV	NIST Webbook
log10ws	-2.35		Crippen Method
logp	2.636		Crippen Method
mcvol	211.880	ml/mol	McGowan Method
pc	2490.03	kPa	Joback Method

tb	933.44	K	Joback Method
tc	1199.86	K	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	34.09	kJ/mol	397.90	NIST Webbook

Sources

Partial Molar Volumes of N,N'-1,2-Ethyl-bis(salicyladimine) Schiff Base (Salen) in Organic Solvents at T = (283.15 to 318.15) K:	https://www.doi.org/10.1021/je100369a
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C94939&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Thermochemical study on the Schiff base[H2salen = N,N -bis(salicylidene) ethylendiamine] and its binuclearcopper (II) complex:	https://www.doi.org/10.1016/j.tca.2013.07.004

Legend

hf:	Enthalpy of formation 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
ie:	Ionization energy
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

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