

Gentisic acid

Other names:

2,5-Dhba
2,5-Dihydroxybenzoic acid
2,5-Dioxybenzoic acid
3,6-Dihydroxybenzoic acid
5-Hydroxysalicylic acid
Benzoic acid, 2,5-dihydroxy-
Gensigen
Gensigon
Gentisate
Gentisinic acid
Hydroquinonecarboxylic acid
Kyselina 2,5-dihydroxybenzoova
Kyselina gentisinova
NSC 27224
Salicylic acid, 5-hydroxy-

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

CAS:

2,5-Dhba
2,5-Dihydroxybenzoic acid
2,5-Dioxybenzoic acid
3,6-Dihydroxybenzoic acid
5-Hydroxysalicylic acid
Benzoic acid, 2,5-dihydroxy-
Gensigen
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Gentisate
Gentisinic acid
Hydroquinonecarboxylic acid
Kyselina 2,5-dihydroxybenzoova
Kyselina gentisinova
NSC 27224
Salicylic acid, 5-hydroxy-

InChI=1S/C7H6O4/c8-4-1-2-6(9)5(3-4)7(10)11/h1-3,8-9H,(H,10,11)

WXTMDXOMEHJXQO-UHFFFAOYSA-N

C5H11NO2

O=C(O)c1cc(O)ccc1O

117.15

490-79-9

Physical Properties

Property code	Value	Unit	Source
affp	531.60 ± 1.30	kJ/mol	NIST Webbook
gf	-454.51	kJ/mol	Joback Method
hf	-570.71	kJ/mol	Joback Method
hfus	20.80	kJ/mol	Vapor Pressures and Enthalpies of Combustion of the Dihydroxybenzoic Acid Isomers
hsub	130.40 ± 1.30	kJ/mol	NIST Webbook
hvap	82.90	kJ/mol	Joback Method
log10ws	-0.11		Aqueous Solubility Prediction Method
logp	0.796		Crippen Method
mcvol	104.910	ml/mol	McGowan Method
pc	8175.04	kPa	Joback Method

tb	693.53	K	Joback Method
tc	922.45	K	Joback Method
tf	476.40	K	Aqueous Solubility Prediction Method
vc	0.277	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	290.73	J/molxK	846.15	Joback Method
cpg	273.90	J/molxK	731.68	Joback Method
cpg	285.24	J/molxK	807.99	Joback Method
cpg	296.25	J/molxK	884.30	Joback Method
cpg	301.93	J/molxK	922.45	Joback Method
cpg	279.67	J/molxK	769.84	Joback Method
cpg	267.80	J/molxK	693.53	Joback Method
dvisc	0.0000136	Paxs	556.64	Joback Method
dvisc	0.0000038	Paxs	611.39	Joback Method
dvisc	0.0000285	Paxs	529.26	Joback Method
dvisc	0.0000021	Paxs	638.77	Joback Method
dvisc	0.0000013	Paxs	666.15	Joback Method
dvisc	0.0000008	Paxs	693.53	Joback Method
dvisc	0.0000069	Paxs	584.02	Joback Method
hfust	20.80	kJ/mol	476.20	NIST Webbook
hsubt	128.10 ± 1.40	kJ/mol	380.50	NIST Webbook
hsubt	117.90 ± 1.40	kJ/mol	370.50	NIST Webbook
psub	2.21e-04	kPa	374.60	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method
psub	1.65e-04	kPa	372.30	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method

psub	1.59e-04	kPa	372.40	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method
psub	2.19e-04	kPa	374.40	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method
psub	2.19e-04	kPa	374.50	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method
psub	1.62e-04	kPa	372.30	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method
psub	2.47e-04	kPa	376.40	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method
psub	2.57e-04	kPa	376.50	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method
psub	2.49e-04	kPa	376.70	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method

psub	2.95e-04	kPa	378.60	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method
psub	3.07e-04	kPa	378.60	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method
psub	2.98e-04	kPa	378.70	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method
psub	1.40e-04	kPa	370.30	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method
psub	1.34e-04	kPa	370.20	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method
psub	1.35e-04	kPa	370.00	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method
psub	1.10e-04	kPa	368.20	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method

psub	1.10e-04	kPa	368.20	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method
psub	1.04e-04	kPa	368.20	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method
psub	8.54e-05	kPa	366.20	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method
psub	8.63e-05	kPa	366.10	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method
psub	8.54e-05	kPa	365.70	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method
psub	6.86e-05	kPa	364.10	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method
psub	7.14e-05	kPa	364.00	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method

psub	5.61e-05	kPa	362.00	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method
psub	5.50e-05	kPa	362.00	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method
psub	5.23e-05	kPa	361.80	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method
psub	6.93e-05	kPa	363.90	Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method

Sources

Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method:

<https://www.doi.org/10.1021/je050293h>

Vapor Pressure Characterization of Several Phenolics and Polyhydric Compounds by Knudsen Effusion Method:

<https://www.doi.org/10.1021/je900777q>

Aqueous Solubility Prediction Method:

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

McGowan Method:

<http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx>

NIST Webbook:

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

Crippen Method:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C490799&Units=SI>

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Legend

affp: Proton affinity
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity

gf:	Standard Gibbs free energy of formation
hf:	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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
psub:	Sublimation pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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