Alizarin

Other names:

1,2-Anthraquinonediol
1,2-Dihydroxy-9,10-anthraquinone
1,2-Dihydroxyanthrachinon
1,2-Dihydroxyanthraquinone
9,10-Anthracenedione, 1,2-dihydroxy-
Alizarin B
Alizarin red
Alizarina
Alizarine
Alizarine 3B
Alizarine B
Alizarine Indicator
Alizarine L Paste
Alizarine Lake Red 2P
Alizarine Lake Red 3P
Alizarine Lake Red IPX
Alizarine NAC
Alizarine Paste 20 percent Bluish
Alizarine Red
Alizarine Red B
Alizarine Red B2
Alizarine Red IP
Alizarine Red IPP
Alizarine Red L
Alizarine paste 20% bluish
Alizerine NAC
Alizerine Red IPP
Anthraquinone, 1,2-dihydroxy-
C.I. 58000
C.I. 58000C
C.I. Mordant Red 11
C.I. Mordant Red 11C
C.I. Pigment Red 83
C.I. Pigment Red 83C
Certiqual Alizarine
Certiqual Alizarine D
D And C Orange Number 15
D and C Orange Number 15D
Deep Crimson Madder 10821
Deep Crimson Madder 10821E

Eljon Madder
Eljon Madder M
Mitsui Alizarine B
Mitsui Alizarine BS
Mordant Red 11
Pincoffin
Sanyo Carmine L2B
Turkey Red
Turkey Red W

Inchi: InChI=1S/C14H8O4/c15-10-6-5-9-11(14(10)18)13(17)8-4-2-1-3-7(8)12(9)16/h1-6,15,18H

InchiKey: RGCKGOZRHPZPFP-UHFFFAOYSA-N

Formula: C14H8O4

SMILES: O=C1c2ccccc2C(=O)c2c1ccc(O)c2O

Mol. weight [g/mol]: 240.21

CAS: 72-48-0

Physical Properties

Property code	Value	Unit	Source
chs	-6062.20	kJ/mol	NIST Webbook
gf	-201.30	kJ/mol	Joback Method
hf	-412.89	kJ/mol	Joback Method
hfus	29.07	kJ/mol	Joback Method
hvap	87.21	kJ/mol	Joback Method
log10ws	-2.78		Aqueous Solubility Prediction Method
logp	1.873		Crippen Method
mcvol	164.620	ml/mol	McGowan Method
pc	4931.51	kPa	Joback Method
tb	887.06	K	Joback Method
tc	1170.41	K	Joback Method
tf	559.32	K	Aqueous Solubility Prediction Method
vc	0.515	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	484.36	J/mol×K	887.06	Joback Method
cpg	496.32	J/mol×K	934.29	Joback Method
cpg	508.20	J/mol×K	981.51	Joback Method
cpg	520.20	J/mol×K	1028.74	Joback Method
cpg	532.57	J/mol×K	1075.96	Joback Method
cpg	545.52	J/mol×K	1123.19	Joback Method
cpg	559.27	J/mol×K	1170.41	Joback Method
hsubt	123.80	kJ/mol	433.00	NIST Webbook
hsubt	121.90 ± 0.50	kJ/mol	469.00	NIST Webbook
hsubt	121.50 ± 0.40	kJ/mol	469.50	NIST Webbook
hsubt	123.90	kJ/mol	403.00	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C72480&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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

hfus: Enthalpy of fusion 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

tb: Normal Boiling Point Temperature

tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume