Indigo

Other names:

Indigotin
CI 73000
3H-Indol-3-one, 2-(1,3-dihydro-3-oxo-2H-indol-2-ylidene)-1,2-dihydro-
«DELTA»2,2'-Bipseudoindoxyl
(«DELTA»2,2'(3H,3'H)-Biindole)-3,3'-dione
(«DELTA»2,2'-Biindoline)-3,3'-dione
Blue No. 201
C.I. Vat Blue 1
C.I. 73000
Cystoceva
D and C Blue No. 6
D and C Blue Number 6
D+C Blue No. 6
D&C Blue No.6
D&C Blue 6
Diindogen
Indigo Blue
Indigo Ciba
Indigo Ciba SL
Indigo J
Indigo N
Indigo NAC
Indigo NACCO
Indigo P
Indigo Powder W
Indigo Pure BASF
Indigo Pure BASF Powder K
Indigo PLN
Indigo Synthetic
Indigo VS
Lithosol Deep Blue B
Mitsui Indigo Paste
Mitsui Indigo Pure
Monolite Fast Navy Blue BV
Pigment Blue 66
Synthetic Indigo
Synthetic Indigo TS
Vat Blue 1
Vulcafix Blue R
Vulcafor Blue A

Vulcanosine Dark Blue L
Vulcol Fast Blue GL
Vynamon Blue A
11669 Blue
(2,2'-Biindoline)-3,3'-dione
Lithosol deep blue V
Modr kypova 1
NCI-C61392
2-(1,3-Dihydro-3-oxo-2H-indol-2-ylidene)-1,2-dihydro-3H-indol-3-one
C.I. pigment blue 66
D & C blue No 6
Indigotine
Indigotin (natural)
Pigment Indigo
2-(1,3-Dihydro-3-oxo-2H-indol-2-ylidene)-1,2-dihydro-3H-indol-3-one (C.I. Vat Blue 1)

Inchi: InChI=1S/C16H10N2O2/c19-15-9-5-1-3-7-11(9)17-13(15)14-16(20)10-6-2-4-8-12(10)18-
InchiKey: COHYTHOBJLSHDF-BUHFOSPRSA-N
Formula: C16H10N2O2
SMILES: O=C1C(=C2Nc3ccccc3C2=O)Nc2ccccc21
Mol. weight [g/mol]: 262.26
CAS: 482-89-3

Physical Properties

Property code	Value	Unit	Source
gf	367.26	kJ/mol	Joback Method
hf	97.89	kJ/mol	Joback Method
hfus	37.27	kJ/mol	Joback Method
hvap	81.16	kJ/mol	Joback Method
log10ws	-4.25		Crippen Method
logp	2.815		Crippen Method
mcvol	185.860	ml/mol	McGowan Method
pc	3585.64	kPa	Joback Method
tb	893.48	K	Joback Method
tc	1183.18	K	Joback Method
tf	764.62	K	Joback Method
vc	0.706	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	595.64	J/mol×K	1134.89	Joback Method
cpg	544.75	J/mol×K	893.48	Joback Method
cpg	557.53	J/mol×K	941.76	Joback Method
cpg	568.94	J/mol×K	990.05	Joback Method
cpg	579.05	J/mol×K	1038.33	Joback Method
cpg	587.93	J/mol×K	1086.61	Joback Method
cpg	602.25	J/mol×K	1183.18	Joback Method
hsubt	136.00	kJ/mol	576.50	NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
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=C482893&Units=SI

Legend

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