Phenolphthalein

Other names:
.alpha, alpha.-Di(p-hydroxyphenyl)phthalide
1(3H)-Isobenzofuranone, 3,3-bis(4-hydroxyphenyl)-
3,3-Bis(4-hydroxyphenyl)-1(3H)-isobenzofuranone
3,3-Bis(4-hydroxyphenyl)-2-benzofuran-1(3h)-one
3,3-Bis(4-hydroxyphenyl)phthalide
3,3-Bis(p-hydroxyphenyl)phthalide
Alophen
Chocolax
Dihydroxyphthalophenone
Doxidan
Espotabs
Euchessina
Evac-Q-Tabs
Evac-Q-kit
Evac-Q-kwik
Evac-U-gen
Ex-Lax
Feen-A-Mint Gum
Feen-A-Mint Laxative Mints
Fenolftalein
Koprol
Laxogen
Lilo
NCI-C55798
NSC 10464
Phenolax
Phenolphthalein,white
Phenolphthalein,yellow
Phenophthalein
Phillips Gelcaps
Phthalide 3,3,-bis(p-hydroxyphenyl)-
Phthalimetten
Phthalin
Purga
Purgen
Purgophen
Spulmako-lax
Trilax
component of Agoral

Inchi:
InChI=1S/C20H14O4/c21-15-9-5-13(6-10-15)20(14-7-11-16(22)12-8-14)18-4-2-1-3-17(18

InchiKey: KJFMBFZCATUALV-UHFFFAOYSA-N
Formula: C20H14O4
SMILES: O=C1OC(c2ccc(O)cc2)(c2ccc(O)cc2)c2ccccc21
Mol. weight [g/mol]: 318.32
CAS: 77-09-8

Physical Properties

Property code	Value	Unit	Source
gf	-17.57	kJ/mol	Joback Method
hf	-294.29	kJ/mol	Joback Method
hfus	40.18	kJ/mol	Joback Method
hvap	101.15	kJ/mol	Joback Method
log10ws	-3.20		Aqueous Solubility Prediction Method
log10ws	-2.90		Estimated Solubility Method
logp	3.560		Crippen Method
mcvol	229.700	ml/mol	McGowan Method
pc	3624.61	kPa	Joback Method
tb	1005.01	K	Joback Method
tc	1299.16	K	Joback Method
tf	535.70 ± 1.50	K	NIST Webbook
tf	534.40	K	Aqueous Solubility Prediction Method
tf	534.70 ± 2.00	K	NIST Webbook
tt	534.00 ± 2.00	K	NIST Webbook
vc	0.747	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	794.43	J/mol×K	1103.06	Joback Method
cpg	823.12	J/mol×K	1152.09	Joback Method
cpg	855.34	J/mol×K	1201.11	Joback Method
cpg	891.69	J/mol×K	1250.14	Joback Method
cpg	745.36	J/mol×K	1005.01	Joback Method
cpg	768.71	J/mol×K	1054.04	Joback Method
cpg	932.73	J/mol×K	1299.16	Joback Method

hfust	51.05	kJ/mol	534.00	NIST Webbook
hfust	51.05	kJ/mol	534.00	NIST Webbook
hfust	51.05	kJ/mol	534.00	NIST Webbook
sfust	95.60	J/mol×K	534.00	NIST Webbook

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C77098&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method: https://en.wikipedia.org/wiki/Joback_method

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
hfust: Enthalpy of fusion 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
sfust: Entropy of fusion at a given temperature
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
tt: Triple Point Temperature
vc: Critical Volume