OXYPHENISATIN ACETATE

Other names:

2-Indolinone, 3,3-bis(p-hydroxyphenyl)-, diacetate (ester)
2H-Indol-2-one, 3,3-bis[4-(acetyloxy)phenyl]-1,3-dihydro-
3,3-Bis(4-acetoxyphenyl)oxindole
3,3-Bis(p-acetoxyphenyl)-2-indolinone
3,3-Bis(p-acetoxyphenyl)oxindole
3,3-Bis(p-hydroxyphenyl)-2-indolinone diacetate
3,3-Bis(p-hydroxyphenyl)-2-indolinone diacetate (ester)
3,3-Bis[4-(acetyloxy)phenyl]-1,3-dihydro-2H-indol-2-one
4,4'-Diacetoxydiphenylisatin
Acelax
Acetalax
Acetophenolisatin
Acetphenolisatin
Bisatin
Brocatine
Bydolax
Cirotyl
Contax
Darmoletten
Diacetoxydiphenylisatin
Diacetyl bis(hydroxyphenyl)isatin
Diacetyl bis(p-hydroxyphenyl)isatin
Diacetyldihydroxydiphenylisatin
Diacetyldioxyphenylisatin
Diacetyldiphenolisatin
Diphesatin
Diphesatine
Eulaxin
Isacen
Isaphen
Isaphenin
Isatin, O,O'-diacetyldiphenol-
Isocrin
Izafenin
LA 96
Lavema
Laxo-Isatin
Laxocol
Lenavac
Lisagal

	NSC 117186
	NSC-59687
	Oxindole, 3,3'-bis(p-hydroxyphenyl)-, diacetate
	Promassolax
	Prulet
	Prulet Liquitab
	Puragaceen
	Purgaceen
	Purgophen
	Sanapert
	Tete-Lax
	oxyphenisatine di(acetate)
Inchi:	InChI=1S/C24H19NO5/c1-15(26)29-19-11-7-17(8-12-19)24(18-9-13-20(14-10-18)30-16(2
InchiKey:	PHPUXYRXPHEJDF-UHFFFAOYSA-N
Formula:	C24H19NO5
SMILES:	CC(=O)Oc1ccc(C2(c3ccc(OC(C)=O)cc3)C(=O)Nc3ccccc32)cc1
Mol. weight [g/mol]:	401.42

Physical Properties

Property code	Value	Unit	Source
hf	-529.76	kJ/mol	Cheméo Relay (1.0)
hfus	45.38	kJ/mol	Joback Method
hvap	126.14	kJ/mol	Cheméo Relay (1.0)
ie	7.51	eV	Cheméo Relay (1.0)
logp	3.824		Crippen Method
mcvol	293.310	ml/mol	McGowan Method
tb	726.16	K	Cheméo Relay (1.0)
tf	524.00 ± 3.00	K	NIST Webbook
tf	516.00 ± 8.00	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	973.89	J/mol×K	1119.43	Joback Method
cpg	992.09	J/mol×K	1165.03	Joback Method
cpg	1010.42	J/mol×K	1210.62	Joback Method
cpg	1029.13	J/mol×K	1256.22	Joback Method

cpg	1048.43	J/mol×K	1301.82	Joback Method
cpg	1068.57	J/mol×K	1347.41	Joback Method
cpg	1089.75	J/mol×K	1393.01	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C115333&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point