Mitotane

Other names:	1,1-Dichloro-2,2-bis(2,4'-dichlorophenyl)ethane 1,1-Dichloro-2-(o-chlorophenyl)-2-(p-chlorophenyl)ethane 1,1-Dichloro-2-(p-chlorophenyl)-2-(o-chlorophenyl)ethane 1,1-dichloro-2-(2-chlorophenyl)-2-(4-chlorophenyl)ethane 1-(2-Chlorophenyl)-1-(4-chlorophenyl)-2,2-dichloroethane 1-(o-Chlorophenyl)-1-(p-chlorophenyl)-2,2-dichloroethane 1-chloro-4-[2,2-dichloro-1-(2-chlorophenyl)ethyl]benzene 2,2-Bis(2-Chlorophenyl-4-chlorophenyl)-1,1-dichloroethane 2,4'-DDD 2,4'-Dichlorodiphenyldichloroethane 2,4'-Dichlorophenyldichlorethane 2-(2-Chlorophenyl)-2-(4-chlorophenyl)-1,1-dichloroethane 2-(o-Chlorophenyl)-2-(p-chlorophenyl)-1,1-dichloroethane Benzene, 1-chloro-2-[2,2-dichloro-1-(4-chlorophenyl)ethyl]- CB 313 Chloditan Chlodithan Chlodithane DDD-o,p' Ethane, 1,1-dichloro-2-(o-chlorophenyl)-2-(p-chlorophenyl)- Ethane, 2-(o-chlorophenyl)-2-(p-chlorophenyl)-1,1-dichloro- Khlodithan Lysodren Mitotan NCI-C04933 NSC-38721 Opeprim ethane, 2,2-dichloro-1-(2-chlorophenyl)-1-(4-chlorophenyl)- o,p'-DDD o,p'-Dichlorodiphenyldichloroethane o,p'-TDE o,p-DDD
Inchi:	InChI=1S/C14H10Cl4/c15-10-7-5-9(6-8-10)13(14(17)18)11-3-1-2-4-12(11)16/h1-8,13-14H
InchiKey:	JWBOIMRXGHLCPP-UHFFFAOYSA-N
Formula:	C14H10Cl4
SMILES:	Clc1ccc(C(c2ccccc2Cl)C(Cl)Cl)cc1
Mol. weight [g/mol]:	320.04
CAS:	53-19-0

Physical Properties

Property code	Value	Unit	Source
gf	219.96	kJ/mol	Joback Method
hf	44.31	kJ/mol	Joback Method
hfus	28.32	kJ/mol	High-pressure phase diagram of the drug mitotane in compressed and/or supercritical CO2
hvap	69.40	kJ/mol	Joback Method
log10ws	-6.51		Aqueous Solubility Prediction Method
log10ws	-6.51		Estimated Solubility Method
logp	5.929		Crippen Method
mcvol	209.560	ml/mol	McGowan Method
pc	2351.92	kPa	Joback Method
rinpol	2146.00		NIST Webbook
rinpol	2130.00		NIST Webbook
rinpol	2119.00		NIST Webbook
rinpol	2146.00		NIST Webbook
rinpol	2123.00		NIST Webbook
rinpol	2118.00		NIST Webbook
rinpol	2130.00		NIST Webbook
rinpol	2119.00		NIST Webbook
rinpol	2130.00		NIST Webbook
rinpol	2116.00		NIST Webbook
rinpol	2128.00		NIST Webbook
rinpol	2119.00		NIST Webbook
rinpol	2123.00		NIST Webbook
rinpol	2116.00		NIST Webbook
rinpol	2128.00		NIST Webbook
rinpol	2118.00		NIST Webbook
rinpol	2118.00		NIST Webbook
rinpol	2123.00		NIST Webbook
ripol	3104.00		NIST Webbook
ripol	3104.00		NIST Webbook
ripol	3120.00		NIST Webbook
ripol	3120.00		NIST Webbook
tb	731.88	K	Joback Method
tc	994.89	K	Joback Method
tf	349.40 ± 0.20	K	NIST Webbook
vc	0.787	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	472.46	J/mol×K	731.88	Joback Method
cpg	484.99	J/mol×K	775.72	Joback Method
cpg	496.33	J/mol×K	819.55	Joback Method
cpg	506.59	J/mol×K	863.39	Joback Method
cpg	515.85	J/mol×K	907.22	Joback Method
cpg	524.22	J/mol×K	951.06	Joback Method
cpg	531.79	J/mol×K	994.89	Joback Method
dvisc	0.0013431	Pa×s	415.10	Joback Method
dvisc	0.0007083	Pa×s	467.90	Joback Method
dvisc	0.0004253	Pa×s	520.69	Joback Method
dvisc	0.0002805	Pa×s	573.49	Joback Method
dvisc	0.0001984	Pa×s	626.29	Joback Method
dvisc	0.0001482	Pa×s	679.08	Joback Method
dvisc	0.0001154	Pa×s	731.88	Joback Method

Sources

High-pressure phase diagram of the drug mitotane in compressed and/or supercritical CO2:	https://www.doi.org/10.1016/j.jct.2009.08.017
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
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=C53190&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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
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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume