Dicofol

Other names:

1,1,1-Trichlor-2,2-bis(4-chlorphenyl)-aethanol
1,1-Bis(4-chlorophenyl)-2,2,2-trichloroethanol
1,1-Bis(p-Chlorophenyl)-2,2,2-trichloroethanol
2,2,2-Trichloor-1,1-bis(4-chloor fenyl)-ethanol
2,2,2-Trichlor-1,1-bis(4-chlor-phenyl)-aethanol
2,2,2-Trichloro-1,1-bis(4-chlorophenyl)ethanol
2,2,2-Trichloro-1,1-bis(4-cloro-fenil)-etanolo
2,2,2-Trichloro-1,1-bis(p-chlorophenyl)ethanol
2,2,2-Trichloro-1,1-di(4-chlorophenyl)ethanol
4,4'-Dichloro-«alpha»-(trichloromethyl)benzhydrol
4-Chloro-«alpha»-(4-chlorophenyl)-«alpha»-(trichloromethyl)benzenemethanol
Acarin
Acetic acid, [3,5-diiodo-4-(4-hydroxy-3-iodophenoxy) phenyl]-, 2-[diethylamino]ethyl ester, hydrochloride
Benzenemethanol, 4-chloro-«alpha»-(4-chlorophenyl)-«alpha»-(trichloromethyl)-
Benzhydrol, 4,4'-dichloro-«alpha»-(trichloromethyl)-
CPCA
Carbax
Cekudifol
DTMC
Decofol
Di-(p-chlorophenyl)trichloromethylcarbinol
Dichlorokelthane
ENT 23,648
Ethanol, 2,2,2-Trichloro-1,1-bis(4-chlorophenyl)-
Ethanol, 2,2,2-trichloro-1,1-bis(p-chlorophenyl)-
Ethanol,1,1-bis(p-chlorophenyl)-2,2,2-trichloro-
FW 293
Fumite Dicofol
Hifol
Hilfol 18.5 EC
Keltane
Kelthane
Kelthane A
Kelthane dust base
Kelthanethanol
Milbol
Mitigan
NCI-C00486
p,p'-Kelthane
p,p-Dicofol

	para,para'-Kelthane
Inchi:	InChI=1S/C14H9Cl5O/c15-11-5-1-9(2-6-11)13(20,14(17,18)19)10-3-7-12(16)8-4-10/h1-8
InchiKey:	UOAMTSKGCBMZTC-UHFFFAOYSA-N
Formula:	C14H9Cl5O
SMILES:	OC(c1ccc(Cl)cc1)(c1ccc(Cl)cc1)C(Cl)(Cl)Cl
Mol. weight [g/mol]:	370.49
CAS:	115-32-2

Physical Properties

Property code	Value	Unit	Source
gf	81.77	kJ/mol	Joback Method
hf	-130.60	kJ/mol	Joback Method
hfus	29.57	kJ/mol	Joback Method
hvap	88.65	kJ/mol	Joback Method
log10ws	-5.67		Estimated Solubility Method
log10ws	-5.67		Aqueous Solubility Prediction Method
logp	5.599		Crippen Method
mcvol	227.670	ml/mol	McGowan Method
pc	2537.93	kPa	Joback Method
ripol	2900.00		NIST Webbook
ripol	2900.00		NIST Webbook
tb	855.91	K	Joback Method
tc	1113.69	K	Joback Method
tf	348.00 ± 0.20	K	NIST Webbook
tf	348.21 ± 0.20	K	NIST Webbook
vc	0.846	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	578.92	J/mol×K	1113.69	Joback Method
cpg	572.34	J/mol×K	1070.72	Joback Method
cpg	565.76	J/mol×K	1027.76	Joback Method
cpg	559.01	J/mol×K	984.80	Joback Method
cpg	551.91	J/mol×K	941.84	Joback Method
cpg	544.31	J/mol×K	898.87	Joback Method

cpg	536.02	J/mol×K	855.91	Joback Method
dvisc	0.0002838	Pa×s	540.68	Joback Method
dvisc	0.0000119	Pa×s	855.91	Joback Method
dvisc	0.0000170	Pa×s	803.37	Joback Method
dvisc	0.0000256	Pa×s	750.83	Joback Method
dvisc	0.0000407	Pa×s	698.30	Joback Method
dvisc	0.0000700	Pa×s	645.76	Joback Method
dvisc	0.0001325	Pa×s	593.22	Joback Method
hfust	19.56	kJ/mol	347.20	NIST Webbook

Sources

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=C115322&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
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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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