

Dichlorophen, O-(cyclobutanecarbonyl)-

Inchi:	InChI=1S/C18H16Cl2O3/c19-14-4-6-16(21)12(9-14)8-13-10-15(20)5-7-17(13)23-18(22)1
InchiKey:	RYAFQLCCJUNCNA-UHFFFAOYSA-N
Formula:	C18H16Cl2O3
SMILES:	O=C(Oc1ccc(Cl)cc1Cc1cc(Cl)ccc1O)C1CCC1
Mol. weight [g/mol]:	351.22

Physical Properties

Property code	Value	Unit	Source
gf	-67.14	kJ/mol	Joback Method
hf	-363.15	kJ/mol	Joback Method
hfus	42.29	kJ/mol	Joback Method
hvap	93.23	kJ/mol	Joback Method
log10ws	-5.71		Crippen Method
logp	4.995		Crippen Method
mcvol	243.890	ml/mol	McGowan Method
pc	2372.59	kPa	Joback Method
rinsol	2834.00		NIST Webbook
tb	922.32	K	Joback Method
tc	1179.46	K	Joback Method
tf	641.16	K	Joback Method
vc	0.865	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	706.37	J/molxK	922.32	Joback Method
cpg	719.57	J/molxK	965.18	Joback Method
cpg	732.09	J/molxK	1008.03	Joback Method
cpg	744.09	J/molxK	1050.89	Joback Method
cpg	755.73	J/molxK	1093.74	Joback Method
cpg	767.16	J/molxK	1136.60	Joback Method
cpg	778.55	J/molxK	1179.46	Joback Method
dvisc	0.0000710	Paxs	641.16	Joback Method
dvisc	0.0000425	Paxs	688.02	Joback Method

dvisc	0.0000271	Paxs	734.88	Joback Method
dvisc	0.0000183	Paxs	781.74	Joback Method
dvisc	0.0000129	Paxs	828.60	Joback Method
dvisc	0.0000094	Paxs	875.46	Joback Method
dvisc	0.0000071	Paxs	922.32	Joback Method

Sources

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=U355166&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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