

Dichlorophen, O-(cyclopropanecarbonyl)-

Inchi:	InChI=1S/C17H14Cl2O3/c18-13-3-5-15(20)11(8-13)7-12-9-14(19)4-6-16(12)22-17(21)10
InchiKey:	GODVCNFGPHZUFN-UHFFFAOYSA-N
Formula:	C17H14Cl2O3
SMILES:	O=C(Oc1ccc(Cl)cc1Cc1cc(Cl)ccc1O)C1CC1
Mol. weight [g/mol]:	337.20

Physical Properties

Property code	Value	Unit	Source
gf	-63.46	kJ/mol	Joback Method
hf	-336.35	kJ/mol	Joback Method
hfus	41.80	kJ/mol	Joback Method
hvap	90.83	kJ/mol	Joback Method
log10ws	-5.29		Crippen Method
logp	4.605		Crippen Method
mcvol	229.800	ml/mol	McGowan Method
pc	2545.61	kPa	Joback Method
rinsol	2737.00		NIST Webbook
tb	895.17	K	Joback Method
tc	1150.38	K	Joback Method
tf	633.41	K	Joback Method
vc	0.817	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	646.49	J/molxK	895.17	Joback Method
cpg	659.02	J/molxK	937.70	Joback Method
cpg	671.00	J/molxK	980.24	Joback Method
cpg	682.58	J/molxK	1022.77	Joback Method
cpg	693.93	J/molxK	1065.31	Joback Method
cpg	705.22	J/molxK	1107.84	Joback Method
cpg	716.60	J/molxK	1150.38	Joback Method
dvisc	0.0001022	Paxs	633.41	Joback Method
dvisc	0.0000645	Paxs	677.04	Joback Method

dvisc	0.0000430	Paxs	720.66	Joback Method
dvisc	0.0000300	Paxs	764.29	Joback Method
dvisc	0.0000218	Paxs	807.92	Joback Method
dvisc	0.0000164	Paxs	851.54	Joback Method
dvisc	0.0000126	Paxs	895.17	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=U354667&Units=SI

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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