Dichlorophen, O,O'-di(cyclopropanecarbonyl)-

Inchi: InChI=1S/C21H18Cl2O4/c22-16-5-7-18(26-20(24)12-1-2-12)14(10-16)9-15-11-17(23)6-8
InchiKey: XYIMISYZCZHNOC-UHFFFAOYSA-N
Formula: C21H18Cl2O4
SMILES: O=C(Oc1ccc(Cl)cc1Cc1cc(Cl)ccc1OC(=O)C1CC1)C1CC1
Mol. weight [g/mol]: 405.27

Physical Properties

Property code	Value	Unit	Source
gf	-57.96	kJ/mol	Joback Method
hf	-425.07	kJ/mol	Joback Method
hfus	46.91	kJ/mol	Joback Method
hvap	96.45	kJ/mol	Joback Method
log10ws	-6.55		Crippen Method
logp	5.215		Crippen Method
mcvol	276.870	ml/mol	McGowan Method
pc	1804.63	kPa	Joback Method
rinpol	2920.00		NIST Webbook
rinpol	2920.00		NIST Webbook
tb	994.08	K	Joback Method
tc	1244.22	K	Joback Method
tf	669.39	K	Joback Method
vc	1.056	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	842.77	J/mol×K	994.08	Joback Method
cpg	855.08	J/mol×K	1035.77	Joback Method
cpg	866.46	J/mol×K	1077.46	Joback Method
cpg	877.02	J/mol×K	1119.15	Joback Method
cpg	886.90	J/mol×K	1160.84	Joback Method
cpg	896.22	J/mol×K	1202.53	Joback Method
cpg	905.09	J/mol×K	1244.22	Joback Method
dvisc	0.0013016	Pa×s	669.39	Joback Method

dvisc	0.0010183	Pa×s	723.50	Joback Method
dvisc	0.0008243	Pa×s	777.62	Joback Method
dvisc	0.0006859	Pa×s	831.73	Joback Method
dvisc	0.0005837	Pa×s	885.85	Joback Method
dvisc	0.0005060	Pa×s	939.96	Joback Method
dvisc	0.0004455	Pa×s	994.08	Joback Method

Sources

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=U354668&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume