Dichlorphen, cyclic ester with dimethylmalonic acid

Inchi: InChI=1S/C18H14Cl2O4/c1-18(2)16(21)23-14-5-3-12(19)8-10(14)7-11-9-13(20)4-6-15(1

InchiKey: FTNIRTALKHVZSM-UHFFFAOYSA-N

Formula: C18H14Cl2O4

SMILES: CC1(C)C(=O)Oc2ccc(Cl)cc2Cc2cc(Cl)ccc2OC1=O

Mol. weight [g/mol]: 365.21

Physical Properties

Property code	Value	Unit	Source
gf	-135.34	kJ/mol	Joback Method
hf	-488.99	kJ/mol	Joback Method
hfus	37.81	kJ/mol	Joback Method
hvap	88.42	kJ/mol	Joback Method
log10ws	-5.64		Crippen Method
logp	4.435		Crippen Method
mcvol	245.460	ml/mol	McGowan Method
pc	2233.41	kPa	Joback Method
rinpol	2617.00		NIST Webbook
tb	968.71	K	Joback Method
tc	1252.10	K	Joback Method
tf	676.24	K	Joback Method
vc	0.912	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	734.29	J/mol×K	968.71	Joback Method
cpg	750.32	J/mol×K	1015.94	Joback Method
cpg	765.60	J/mol×K	1063.17	Joback Method
cpg	780.28	J/mol×K	1110.41	Joback Method
cpg	794.52	J/mol×K	1157.64	Joback Method
cpg	808.46	J/mol×K	1204.87	Joback Method
cpg	822.25	J/mol×K	1252.10	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U363643&Units=SI

Legend

cpg:	Ideal gas heat capacity
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