Dichlorophen, O-(3-methylbut-2-enoyl)-

Inchi: InChI=1S/C18H16Cl2O3/c1-11(2)7-18(22)23-17-6-4-15(20)10-13(17)8-12-9-14(19)3-5-16
InchiKey: RHKPGIBQSRHTSC-UHFFFAOYSA-N
Formula: C18H16Cl2O3
SMILES: CC(C)=CC(=O)Oc1ccc(Cl)cc1Cc1cc(Cl)ccc1O
Mol. weight [g/mol]: 351.22

Physical Properties

Property code	Value	Unit	Source
gf	-44.12	kJ/mol	Joback Method
hf	-322.36	kJ/mol	Joback Method
hfus	45.15	kJ/mol	Joback Method
hvap	93.18	kJ/mol	Joback Method
log10ws	-5.91		Crippen Method
logp	5.161		Crippen Method
mcvol	250.450	ml/mol	McGowan Method
pc	2161.32	kPa	Joback Method
rinpol	2771.00		NIST Webbook
tb	915.35	K	Joback Method
tc	1164.82	K	Joback Method
tf	607.70	K	Joback Method
vc	0.896	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	692.54	J/mol×K	915.35	Joback Method
cpg	705.05	J/mol×K	956.93	Joback Method
cpg	717.00	J/mol×K	998.51	Joback Method
cpg	728.52	J/mol×K	1040.08	Joback Method
cpg	739.74	J/mol×K	1081.66	Joback Method
cpg	750.80	J/mol×K	1123.24	Joback Method
cpg	761.85	J/mol×K	1164.82	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355134&Units=SI
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

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