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

Inchi: InChI=1S/C21H22Cl2O4/c1-12(2)20(24)26-18-7-5-16(22)10-14(18)9-15-11-17(23)6-8-19
InchiKey: NYZJHKVEYLEUNQ-UHFFFAOYSA-N
Formula: C21H22Cl2O4
SMILES: CC(C)C(=O)Oc1ccc(Cl)cc1Cc1cc(Cl)ccc1OC(=O)C(C)C
Mol. weight [g/mol]: 409.30

Physical Properties

Property code	Value	Unit	Source
gf	-184.34	kJ/mol	Joback Method
hf	-581.23	kJ/mol	Joback Method
hfus	43.59	kJ/mol	Joback Method
hvap	95.85	kJ/mol	Joback Method
log10ws	-6.76		Crippen Method
logp	5.707		Crippen Method
mcvol	298.590	ml/mol	McGowan Method
pc	1481.57	kPa	Joback Method
rinpol	2640.00		NIST Webbook
tb	979.72	K	Joback Method
tc	1217.09	K	Joback Method
tf	603.51	K	Joback Method
vc	1.129	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	880.25	J/mol×K	979.72	Joback Method
cpg	922.30	J/mol×K	1177.53	Joback Method
cpg	916.64	J/mol×K	1137.97	Joback Method
cpg	909.63	J/mol×K	1098.41	Joback Method
cpg	901.25	J/mol×K	1058.84	Joback Method
cpg	891.47	J/mol×K	1019.28	Joback Method
cpg	926.65	J/mol×K	1217.09	Joback Method
dvisc	0.0000318	Pa×s	979.72	Joback Method
dvisc	0.0000401	Pa×s	917.02	Joback Method

dvisc	0.0000522	Pa×s	854.32	Joback Method
dvisc	0.0000709	Pa×s	791.62	Joback Method
dvisc	0.0001015	Pa×s	728.91	Joback Method
dvisc	0.0001556	Pa×s	666.21	Joback Method
dvisc	0.0002604	Pa×s	603.51	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=U354644&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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