Dichlorophen, O,O'-di(4-methylbenzoyl)-

Inchi: InChI=1S/C29H22Cl2O4/c1-18-3-7-20(8-4-18)28(32)34-26-13-11-24(30)16-22(26)15-23-
InchiKey: PHHBCNJGNQBPRS-UHFFFAOYSA-N
Formula: C29H22Cl2O4
SMILES: Cc1ccc(C(=O)Oc2ccc(Cl)cc2Cc2cc(Cl)ccc2OC(=O)c2ccc(C)cc2)cc1
Mol. weight [g/mol]: 505.39

Physical Properties

Property code	Value	Unit	Source
gf	93.46	kJ/mol	Joback Method
hf	-285.67	kJ/mol	Joback Method
hfus	58.66	kJ/mol	Joback Method
hvap	120.31	kJ/mol	Joback Method
log10ws	-10.07		Crippen Method
logp	7.639		Crippen Method
mcvol	363.790	ml/mol	McGowan Method
pc	1322.31	kPa	Joback Method
rinpol	3312.00		NIST Webbook
rinpol	3312.00		NIST Webbook
tb	1226.96	K	Joback Method
tc	1506.22	K	Joback Method
tf	801.55	K	Joback Method
vc	1.373	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1105.04	J/mol×K	1226.96	Joback Method
cpg	1109.78	J/mol×K	1273.50	Joback Method
cpg	1112.86	J/mol×K	1320.05	Joback Method
cpg	1114.40	J/mol×K	1366.59	Joback Method
cpg	1114.49	J/mol×K	1413.13	Joback Method
cpg	1113.24	J/mol×K	1459.67	Joback Method
cpg	1110.77	J/mol×K	1506.22	Joback Method
dvisc	0.0000750	Pa×s	801.55	Joback Method

dvisc	0.0000503	Pa×s	872.45	Joback Method
dvisc	0.0000358	Pa×s	943.35	Joback Method
dvisc	0.0000267	Pa×s	1014.26	Joback Method
dvisc	0.0000207	Pa×s	1085.16	Joback Method
dvisc	0.0000166	Pa×s	1156.06	Joback Method
dvisc	0.0000136	Pa×s	1226.96	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=U354160&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