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

Inchi: InChI=1S/C27H30Cl2O4/c28-22-11-13-24(32-26(30)18-7-3-1-4-8-18)20(16-22)15-21-17-
InchiKey: WVXRRQFYHHDBJY-UHFFFAOYSA-N
Formula: C27H30Cl2O4
SMILES: O=C(Oc1ccc(Cl)cc1Cc1cc(Cl)ccc1OC(=O)C1CCCCC1)C1CCCCC1
Mol. weight [g/mol]: 489.43

Physical Properties

Property code	Value	Unit	Source
gf	-80.04	kJ/mol	Joback Method
hf	-585.87	kJ/mol	Joback Method
hfus	49.85	kJ/mol	Joback Method
hvap	110.84	kJ/mol	Joback Method
log10ws	-9.06		Crippen Method
logp	7.556		Crippen Method
mcvol	361.410	ml/mol	McGowan Method
pc	1293.93	kPa	Joback Method
rinpol	3571.00		NIST Webbook
rinpol	3571.00		NIST Webbook
tb	1156.98	K	Joback Method
tc	1425.92	K	Joback Method
tf	715.89	K	Joback Method
vc	1.343	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1211.15	J/mol×K	1156.98	Joback Method
cpg	1228.00	J/mol×K	1381.10	Joback Method
cpg	1228.81	J/mol×K	1336.28	Joback Method
cpg	1227.63	J/mol×K	1291.45	Joback Method
cpg	1224.35	J/mol×K	1246.63	Joback Method
cpg	1218.89	J/mol×K	1201.80	Joback Method
cpg	1225.29	J/mol×K	1425.92	Joback Method
dvisc	0.0000162	Pa×s	1156.98	Joback Method

dvisc	0.0000205	Pa×s	1083.46	Joback Method
dvisc	0.0000269	Pa×s	1009.95	Joback Method
dvisc	0.0000368	Pa×s	936.43	Joback Method
dvisc	0.0000532	Pa×s	862.92	Joback Method
dvisc	0.0000823	Pa×s	789.40	Joback Method
dvisc	0.0001393	Pa×s	715.89	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354657&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

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

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