

Dichlorphen, O,O'-dibenzoyl-

Inchi:	InChI=1S/C27H18Cl2O4/c28-22-11-13-24(32-26(30)18-7-3-1-4-8-18)20(16-22)15-21-17-
InchiKey:	QFVWZPUVNBKTBQA-UHFFFAOYSA-N
Formula:	C27H18Cl2O4
SMILES:	O=C(Oc1ccc(Cl)cc1Cc1cc(Cl)ccc1OC(=O)c1ccccc1)c1ccccc1
Mol. weight [g/mol]:	477.33

Physical Properties

Property code	Value	Unit	Source
gf	95.88	kJ/mol	Joback Method
hf	-221.45	kJ/mol	Joback Method
hfus	54.26	kJ/mol	Joback Method
hvap	114.53	kJ/mol	Joback Method
log10ws	-9.12		Crippen Method
logp	7.023		Crippen Method
mcvol	335.610	ml/mol	McGowan Method
pc	1564.75	kPa	Joback Method
rinsol	2584.00		NIST Webbook
tb	1171.24	K	Joback Method
tc	1447.46	K	Joback Method
tf	753.97	K	Joback Method
vc	1.262	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	994.15	J/molxK	1171.24	Joback Method
cpg	1010.17	J/molxK	1401.43	Joback Method
cpg	1009.39	J/molxK	1355.39	Joback Method
cpg	1007.52	J/molxK	1309.35	Joback Method
cpg	1004.44	J/molxK	1263.31	Joback Method
cpg	1000.02	J/molxK	1217.28	Joback Method
cpg	1009.97	J/molxK	1447.46	Joback Method
dvisc	0.0000172	Paxs	1171.24	Joback Method
dvisc	0.0000211	Paxs	1101.70	Joback Method

dvisc	0.0000268	Paxs	1032.15	Joback Method
dvisc	0.0000351	Paxs	962.61	Joback Method
dvisc	0.0000479	Paxs	893.06	Joback Method
dvisc	0.0000690	Paxs	823.52	Joback Method
dvisc	0.0001064	Paxs	753.97	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=U360689&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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

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