Dichlorphen, O,O'-di(pentafluorobenzoyl)-

Inchi: InChI=1S/C27H8Cl2F10O4/c28-10-1-3-12(42-26(40)14-16(30)20(34)24(38)21(35)17(14)
InchiKey: CDEGXIKTBLFWRO-UHFFFAOYSA-N
Formula: C27H8Cl2F10O4
SMILES: O=C(Oc1ccc(Cl)cc1Cc1cc(Cl)ccc1OC(=O)c1c(F)c(F)c(F)c(F)c1F)c1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 657.24

Physical Properties

Property code	Value	Unit	Source
gf	-1948.52	kJ/mol	Joback Method
hf	-2297.25	kJ/mol	Joback Method
hfus	81.17	kJ/mol	Joback Method
hvap	112.98	kJ/mol	Joback Method
log10ws	-12.43		Crippen Method
logp	8.414		Crippen Method
mcvol	353.310	ml/mol	McGowan Method
pc	1022.04	kPa	Joback Method
rinpol	3003.00		NIST Webbook
rinpol	3003.00		NIST Webbook
tb	1213.74	K	Joback Method
tc	1499.09	K	Joback Method
tf	885.07	K	Joback Method
vc	1.442	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1025.49	J/mol×K	1213.74	Joback Method
cpg	1024.89	J/mol×K	1261.30	Joback Method
cpg	1021.84	J/mol×K	1308.86	Joback Method
cpg	1016.36	J/mol×K	1356.42	Joback Method
cpg	1008.46	J/mol×K	1403.98	Joback Method
cpg	998.13	J/mol×K	1451.53	Joback Method
cpg	985.39	J/mol×K	1499.09	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=U360634&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
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