Dichlorphen, O,O'-bis(3-Fluoro-4-trifluoromethylbenzoyl)-

Inchi: InChI=1S/C29H14Cl2F8O4/c30-18-3-7-24(42-26(40)14-1-5-20(22(32)12-14)28(34,35)36)
InchiKey: RDVVZTBMYULZEL-UHFFFAOYSA-N
Formula: C29H14Cl2F8O4
SMILES: O=C(Oc1ccc(Cl)cc1Cc1cc(Cl)ccc1OC(=O)c1ccc(C(F)(F)F)c(F)c1)c1ccc(C(F)(F)F)c(F)c1
Mol. weight [g/mol]: 649.31

Physical Properties

Property code	Value	Unit	Source
gf	-1478.60	kJ/mol	Joback Method
hf	-1894.99	kJ/mol	Joback Method
hfus	67.70	kJ/mol	Joback Method
hvap	112.50	kJ/mol	Joback Method
log10ws	-11.99		Crippen Method
logp	9.338		Crippen Method
mcvol	377.950	ml/mol	McGowan Method
pc	1039.24	kPa	Joback Method
rinpol	3214.00		NIST Webbook
tb	1224.62	K	Joback Method
tc	1502.10	K	Joback Method
tf	836.15	K	Joback Method
vc	1.496	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1155.02	J/mol×K	1224.62	Joback Method
cpg	1160.97	J/mol×K	1270.87	Joback Method
cpg	1166.10	J/mol×K	1317.11	Joback Method
cpg	1170.57	J/mol×K	1363.36	Joback Method
cpg	1174.59	J/mol×K	1409.61	Joback Method
cpg	1178.33	J/mol×K	1455.86	Joback Method
cpg	1181.99	J/mol×K	1502.10	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360603&Units=SI

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