Dichlorphen, O,O'-bis(2,4-difluorobenzoyl)-

Inchi: InChI=1S/C27H14Cl2F4O4/c28-16-1-7-24(36-26(34)20-5-3-18(30)12-22(20)32)14(10-16
InchiKey: GPBZIHDMTFKGCX-UHFFFAOYSA-N
Formula: C27H14Cl2F4O4
SMILES: O=C(Oc1ccc(Cl)cc1Cc1cc(Cl)ccc1OC(=O)c1ccc(F)cc1F)c1ccc(F)cc1F
Mol. weight [g/mol]: 549.30

Physical Properties

Property code	Value	Unit	Source
gf	-721.88	kJ/mol	Joback Method
hf	-1051.77	kJ/mol	Joback Method
hfus	65.03	kJ/mol	Joback Method
hvap	113.91	kJ/mol	Joback Method
log10ws	-10.44		Crippen Method
logp	7.579		Crippen Method
mcvol	342.690	ml/mol	McGowan Method
pc	1305.17	kPa	Joback Method
rinpol	3396.00		NIST Webbook
tb	1188.24	K	Joback Method
tc	1455.36	K	Joback Method
tf	806.41	K	Joback Method
vc	1.333	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1007.82	J/mol×K	1188.24	Joback Method
cpg	1011.21	J/mol×K	1232.76	Joback Method
cpg	1012.96	J/mol×K	1277.28	Joback Method
cpg	1013.12	J/mol×K	1321.80	Joback Method
cpg	1011.77	J/mol×K	1366.32	Joback Method
cpg	1008.97	J/mol×K	1410.84	Joback Method
cpg	1004.79	J/mol×K	1455.36	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=U360566&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