Dichlorophen, O,O'-di(3-fluorobenzoyl)-

Inchi: InChI=1S/C27H16Cl2F2O4/c28-20-7-9-24(34-26(32)16-3-1-5-22(30)14-16)18(12-20)11-1
InchiKey: MYDYUTGBFCPIPM-UHFFFAOYSA-N
Formula: C27H16Cl2F2O4
SMILES: O=C(Oc1ccc(Cl)cc1Cc1cc(Cl)ccc1OC(=O)c1cccc(F)c1)c1cccc(F)c1
Mol. weight [g/mol]: 513.32

Physical Properties

Property code	Value	Unit	Source
gf	-313.00	kJ/mol	Joback Method
hf	-636.61	kJ/mol	Joback Method
hfus	59.64	kJ/mol	Joback Method
hvap	114.22	kJ/mol	Joback Method
log10ws	-9.78		Crippen Method
logp	7.301		Crippen Method
mcvol	339.150	ml/mol	McGowan Method
pc	1426.15	kPa	Joback Method
rinpol	3524.00		NIST Webbook
rinpol	3524.00		NIST Webbook
tb	1179.74	K	Joback Method
tc	1449.32	K	Joback Method
tf	780.19	K	Joback Method
vc	1.298	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1001.17	J/mol×K	1179.74	Joback Method
cpg	1005.77	J/mol×K	1224.67	Joback Method
cpg	1008.85	J/mol×K	1269.60	Joback Method
cpg	1010.50	J/mol×K	1314.53	Joback Method
cpg	1010.79	J/mol×K	1359.46	Joback Method
cpg	1009.82	J/mol×K	1404.39	Joback Method
cpg	1007.69	J/mol×K	1449.32	Joback Method

Sources

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=U355670&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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