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

Inchi: InChI=1S/C29H16Cl2F6O4/c30-22-7-9-24(40-26(38)16-3-1-5-20(12-16)28(32,33)34)18(1

InchiKey: NWSJXVYBCWVKAI-UHFFFAOYSA-N

Formula: C29H16Cl2F6O4

SMILES: O=C(Oc1ccc(Cl)cc1Cc1cc(Cl)ccc1OC(=O)c1cccc(C(F)(F)F)c1)c1cccc(C(F)(F)F)c1

Mol. weight [g/mol]: 613.33

Physical Properties

Property code	Value	Unit	Source
gf	-1069.72	kJ/mol	Joback Method
hf	-1479.83	kJ/mol	Joback Method
hfus	62.32	kJ/mol	Joback Method
hvap	112.81	kJ/mol	Joback Method
log10ws	-11.32		Crippen Method
logp	9.060		Crippen Method
mcvol	374.410	ml/mol	McGowan Method
pc	1124.57	kPa	Joback Method
rinpol	3316.00		NIST Webbook
rinpol	3316.00		NIST Webbook
tb	1216.12	K	Joback Method
tc	1488.91	K	Joback Method
tf	809.93	K	Joback Method
vc	1.460	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1148.69	J/mol×K	1216.12	Joback Method
cpg	1155.74	J/mol×K	1261.59	Joback Method
cpg	1162.12	J/mol×K	1307.05	Joback Method
cpg	1168.05	J/mol×K	1352.52	Joback Method
cpg	1173.72	J/mol×K	1397.98	Joback Method
cpg	1179.33	J/mol×K	1443.45	Joback Method
cpg	1185.09	J/mol×K	1488.91	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=U355149&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