Dichlorophen, O-(2-trifluoromethylbenzoyl)-

Inchi: InChI=1S/C21H13Cl2F3O3/c22-14-5-7-18(27)12(10-14)9-13-11-15(23)6-8-19(13)29-20(2
InchiKey: QXKLLOALYRKGCX-UHFFFAOYSA-N
Formula: C21H13Cl2F3O3
SMILES: O=C(Oc1ccc(Cl)cc1Cc1cc(Cl)ccc1O)c1ccccc1C(F)(F)F
Mol. weight [g/mol]: 441.23

Physical Properties

Property code	Value	Unit	Source
gf	-569.34	kJ/mol	Joback Method
hf	-863.73	kJ/mol	Joback Method
hfus	49.50	kJ/mol	Joback Method
hvap	99.01	kJ/mol	Joback Method
log10ws	-7.68		Crippen Method
logp	6.528		Crippen Method
mcvol	278.570	ml/mol	McGowan Method
pc	1896.95	kPa	Joback Method
rinpol	3043.00		NIST Webbook
rinpol	3043.00		NIST Webbook
tb	1006.19	K	Joback Method
tc	1256.83	K	Joback Method
tf	703.68	K	Joback Method
vc	1.018	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	805.84	J/mol×K	1006.19	Joback Method
cpg	816.89	J/mol×K	1047.96	Joback Method
cpg	827.58	J/mol×K	1089.74	Joback Method
cpg	838.09	J/mol×K	1131.51	Joback Method
cpg	848.59	J/mol×K	1173.29	Joback Method
cpg	859.25	J/mol×K	1215.06	Joback Method
cpg	870.24	J/mol×K	1256.83	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355161&Units=SI
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

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