Fumaric acid, 2-isopropylphenyl 2,4,6-trichlorophenyl ester

Inchi: InChI=1S/C19H15Cl3O4/c1-11(2)13-5-3-4-6-16(13)25-17(23)7-8-18(24)26-19-14(21)9-12
InchiKey: LNYOMCCTXRXPMO-BQYQJAHWSA-N
Formula: C19H15Cl3O4
SMILES: CC(C)c1ccccc1OC(=O)C=CC(=O)Oc1c(Cl)cc(Cl)cc1Cl
Mol. weight [g/mol]: 413.68

Physical Properties

Property code	Value	Unit	Source
gf	-130.45	kJ/mol	Joback Method
hf	-433.19	kJ/mol	Joback Method
hfus	46.34	kJ/mol	Joback Method
hvap	96.12	kJ/mol	Joback Method
log10ws	-6.84		Crippen Method
logp	5.837		Crippen Method
mcvol	278.350	ml/mol	McGowan Method
pc	1737.56	kPa	Joback Method
rinpol	2736.00		NIST Webbook
rinpol	2736.00		NIST Webbook
tb	975.99	K	Joback Method
tc	1222.57	K	Joback Method
tf	620.81	K	Joback Method
vc	1.052	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	754.45	J/mol×K	975.99	Joback Method
cpg	763.96	J/mol×K	1017.09	Joback Method
cpg	772.28	J/mol×K	1058.18	Joback Method
cpg	779.48	J/mol×K	1099.28	Joback Method
cpg	785.58	J/mol×K	1140.38	Joback Method
cpg	790.65	J/mol×K	1181.47	Joback Method
cpg	794.72	J/mol×K	1222.57	Joback Method
dvisc	0.0002318	Pa×s	620.81	Joback Method

dvisc	0.0001474	Pa×s	680.01	Joback Method
dvisc	0.0001008	Pa×s	739.20	Joback Method
dvisc	0.0000730	Pa×s	798.40	Joback Method
dvisc	0.0000552	Pa×s	857.60	Joback Method
dvisc	0.0000433	Pa×s	916.79	Joback Method
dvisc	0.0000350	Pa×s	975.99	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=U405872&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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