Fumaric acid, 2-isopropoxyphenyl 3-chlorophenyl ester

Inchi: InChI=1S/C19H17ClO5/c1-13(2)23-16-8-3-4-9-17(16)25-19(22)11-10-18(21)24-15-7-5-6-

InchiKey: YOTRBBPIXZZBIE-ZHACJKMWSA-N

Formula: C19H17ClO5

SMILES: CC(C)Oc1ccccc1OC(=O)C=CC(=O)Oc1cccc(Cl)c1

Mol. weight [g/mol]: 360.79

Physical Properties

Property code	Value	Unit	Source
gf	-192.33	kJ/mol	Joback Method
hf	-510.99	kJ/mol	Joback Method
hfus	39.91	kJ/mol	Joback Method
hvap	88.44	kJ/mol	Joback Method
log10ws	-5.36		Crippen Method
logp	4.194		Crippen Method
mcvol	259.740	ml/mol	McGowan Method
pc	1870.79	kPa	Joback Method
rinpol	2563.00		NIST Webbook
rinpol	2563.00		NIST Webbook
tb	913.59	K	Joback Method
tc	1151.23	K	Joback Method
tf	558.16	K	Joback Method
vc	0.973	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	744.58	J/mol×K	913.59	Joback Method
cpg	756.18	J/mol×K	953.20	Joback Method
cpg	766.46	J/mol×K	992.80	Joback Method
cpg	775.46	J/mol×K	1032.41	Joback Method
cpg	783.22	J/mol×K	1072.01	Joback Method
cpg	789.75	J/mol×K	1111.62	Joback Method
cpg	795.11	J/mol×K	1151.23	Joback Method
dvisc	0.0002973	Pa×s	558.16	Joback Method

dvisc	0.0001743	Pa×s	617.40	Joback Method
dvisc	0.0001122	Pa×s	676.64	Joback Method
dvisc	0.0000775	Pa×s	735.88	Joback Method
dvisc	0.0000566	Pa×s	795.11	Joback Method
dvisc	0.0000431	Pa×s	854.35	Joback Method
dvisc	0.0000341	Pa×s	913.59	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=U405714&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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