Fumaric acid, 2-isopropylphenyl 2,3-dichlorophenyl ester

Inchi: InChI=1S/C19H16Cl2O4/c1-12(2)13-6-3-4-8-15(13)24-17(22)10-11-18(23)25-16-9-5-7-14

InchiKey: GNFJDVWCHMHXRG-ZHACJKMWSA-N

Formula: C19H16Cl2O4

SMILES: CC(C)c1ccccc1OC(=O)C=CC(=O)Oc1cccc(Cl)c1Cl

Mol. weight [g/mol]: 379.23

Physical Properties

Property code	Value	Unit	Source
gf	-108.89	kJ/mol	Joback Method
hf	-405.98	kJ/mol	Joback Method
hfus	42.53	kJ/mol	Joback Method
hvap	91.08	kJ/mol	Joback Method
log10ws	-6.16		Crippen Method
logp	5.184		Crippen Method
mcvol	266.110	ml/mol	McGowan Method
pc	1815.41	kPa	Joback Method
rinpol	2693.00		NIST Webbook
rinpol	2693.00		NIST Webbook
tb	933.58	K	Joback Method
tc	1176.51	K	Joback Method
tf	578.37	K	Joback Method
vc	1.004	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	737.65	J/mol×K	933.58	Joback Method
cpg	748.56	J/mol×K	974.07	Joback Method
cpg	758.28	J/mol×K	1014.56	Joback Method
cpg	766.86	J/mol×K	1055.04	Joback Method
cpg	774.34	J/mol×K	1095.53	Joback Method
cpg	780.78	J/mol×K	1136.02	Joback Method
cpg	786.24	J/mol×K	1176.51	Joback Method
dvisc	0.0003088	Pa×s	578.37	Joback Method

dvisc	0.0001875	Pa×s	637.57	Joback Method
dvisc	0.0001240	Pa×s	696.77	Joback Method
dvisc	0.0000874	Pa×s	755.97	Joback Method
dvisc	0.0000649	Pa×s	815.18	Joback Method
dvisc	0.0000501	Pa×s	874.38	Joback Method
dvisc	0.0000400	Pa×s	933.58	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=U405870&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