Fumaric acid, 2-isopropoxyphenyl 2,2-dichloroethyl ester

Inchi: InChI=1S/C15H16Cl2O5/c1-10(2)21-11-5-3-4-6-12(11)22-15(19)8-7-14(18)20-9-13(16)17

InchiKey: SIPTYGJDQSDZJZ-BQYQJAHWSA-N

Formula: C15H16Cl2O5

SMILES: CC(C)Oc1ccccc1OC(=O)C=CC(=O)OCC(Cl)Cl

Mol. weight [g/mol]: 347.19

Physical Properties

Property code	Value	Unit	Source
gf	-343.16	kJ/mol	Joback Method
hf	-674.51	kJ/mol	Joback Method
hfus	36.57	kJ/mol	Joback Method
hvap	80.60	kJ/mol	Joback Method
log10ws	-4.16		Crippen Method
logp	3.282		Crippen Method
mcvol	239.380	ml/mol	McGowan Method
pc	1935.54	kPa	Joback Method
rinpol	2226.00		NIST Webbook
rinpol	2226.00		NIST Webbook
tb	827.40	K	Joback Method
tc	1049.22	K	Joback Method
tf	489.06	K	Joback Method
vc	0.899	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	645.48	J/mol×K	827.40	Joback Method
cpg	694.67	J/mol×K	1012.25	Joback Method
cpg	686.89	J/mol×K	975.28	Joback Method
cpg	678.10	J/mol×K	938.31	Joback Method
cpg	668.27	J/mol×K	901.34	Joback Method
cpg	657.41	J/mol×K	864.37	Joback Method
cpg	701.45	J/mol×K	1049.22	Joback Method
dvisc	0.0000457	Pa×s	827.40	Joback Method

dvisc	0.0000593	Pa×s	771.01	Joback Method
dvisc	0.0000803	Pa×s	714.62	Joback Method
dvisc	0.0001145	Pa×s	658.23	Joback Method
dvisc	0.0001744	Pa×s	601.84	Joback Method
dvisc	0.0002900	Pa×s	545.45	Joback Method
dvisc	0.0005419	Pa×s	489.06	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=U405711&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