

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

Inchi:	InChI=1S/C19H16Cl2O5/c1-12(2)24-14-7-3-4-8-15(14)25-17(22)10-11-18(23)26-16-9-5-6
InchiKey:	OGILBBGEWOFQRZ-ZHACJKMWSA-N
Formula:	C19H16Cl2O5
SMILES:	CC(C)Oc1ccccc1OC(=O)C=CC(=O)Oc1cccc(Cl)c1Cl
Mol. weight [g/mol]:	395.23

Physical Properties

Property code	Value	Unit	Source
gf	-213.89	kJ/mol	Joback Method
hf	-538.20	kJ/mol	Joback Method
hfus	43.72	kJ/mol	Joback Method
hvap	93.49	kJ/mol	Joback Method
log10ws	-6.04		Crippen Method
logp	4.848		Crippen Method
mcvol	271.980	ml/mol	McGowan Method
pc	1789.39	kPa	Joback Method
tb	956.00	K	Joback Method
tc	1197.45	K	Joback Method
tf	600.60	K	Joback Method
vc	1.022	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	762.49	J/molxK	956.00	Joback Method
cpg	799.84	J/molxK	1157.21	Joback Method
cpg	794.90	J/molxK	1116.97	Joback Method
cpg	788.73	J/molxK	1076.72	Joback Method
cpg	781.28	J/molxK	1036.48	Joback Method
cpg	772.55	J/molxK	996.24	Joback Method
cpg	803.58	J/molxK	1197.45	Joback Method
dvisc	0.0000298	Paxs	956.00	Joback Method
dvisc	0.0000372	Paxs	896.77	Joback Method
dvisc	0.0000480	Paxs	837.53	Joback Method

dvisc	0.0000644	Paxs	778.30	Joback Method
dvisc	0.0000906	Paxs	719.07	Joback Method
dvisc	0.0001356	Paxs	659.83	Joback Method
dvisc	0.0002197	Paxs	600.60	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405715&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvac:	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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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