Fumaric acid, 2-isopropoxyphenyl 8-chlorooctyl ester

Inchi: InChI=1S/C21H29ClO5/c1-17(2)26-18-11-7-8-12-19(18)27-21(24)14-13-20(23)25-16-10-

InchiKey: PFPALQAZHAFJKV-BUHFOSPRSA-N

Formula: C21H29ClO5

SMILES: CC(C)Oc1ccccc1OC(=O)C=CC(=O)OCCCCCCCCCl

Mol. weight [g/mol]: 396.90

Physical Properties

Property code	Value	Unit	Source
gf	-278.27	kJ/mol	Joback Method
hf	-777.33	kJ/mol	Joback Method
hfus	51.44	kJ/mol	Joback Method
hvap	89.95	kJ/mol	Joback Method
log10ws	-5.91		Crippen Method
logp	5.058		Crippen Method
mcvol	311.680	ml/mol	McGowan Method
pc	1257.48	kPa	Joback Method
rinpol	2835.00		NIST Webbook
rinpol	2835.00		NIST Webbook
tb	927.69	K	Joback Method
tc	1141.23	K	Joback Method
tf	541.76	K	Joback Method
vc	1.192	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	965.34	J/mol×K	927.69	Joback Method
cpg	979.57	J/mol×K	963.28	Joback Method
cpg	992.55	J/mol×K	998.87	Joback Method
cpg	1004.30	J/mol×K	1034.46	Joback Method
cpg	1014.86	J/mol×K	1070.05	Joback Method
cpg	1024.27	J/mol×K	1105.64	Joback Method
cpg	1032.54	J/mol×K	1141.23	Joback Method
dvisc	0.0003084	Pa×s	541.76	Joback Method

dvisc	0.0001611	Pa×s	606.08	Joback Method
dvisc	0.0000953	Pa×s	670.40	Joback Method
dvisc	0.0000619	Pa×s	734.72	Joback Method
dvisc	0.0000430	Pa×s	799.05	Joback Method
dvisc	0.0000316	Pa×s	863.37	Joback Method
dvisc	0.0000242	Pa×s	927.69	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405716&Units=SI
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

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