Fumaric acid, 3-phenylpropyl 3-chlorophenyl ester

Inchi: InChI=1S/C19H17ClO4/c20-16-9-4-10-17(14-16)24-19(22)12-11-18(21)23-13-5-8-15-6-2

InchiKey: XQPMESFBMBVCSK-VAWYXSNFSA-N

Formula: C19H17ClO4

SMILES: O=C(C=CC(=O)Oc1cccc(Cl)c1)OCCCc1ccccc1

Mol. weight [g/mol]: 344.79

Physical Properties

Property code	Value	Unit	Source
gf	-75.26	kJ/mol	Joback Method
hf	-362.02	kJ/mol	Joback Method
hfus	42.63	kJ/mol	Joback Method
hvap	85.76	kJ/mol	Joback Method
log10ws	-4.89		Crippen Method
logp	3.978		Crippen Method
mcvol	253.870	ml/mol	McGowan Method
pc	1910.24	kPa	Joback Method
rinpol	2666.00		NIST Webbook
rinpol	2666.00		NIST Webbook
tb	886.63	K	Joback Method
tc	1122.07	K	Joback Method
tf	538.41	K	Joback Method
vc	0.961	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	719.77	J/mol×K	886.63	Joback Method
cpg	732.08	J/mol×K	925.87	Joback Method
cpg	743.22	J/mol×K	965.11	Joback Method
cpg	753.25	J/mol×K	1004.35	Joback Method
cpg	762.25	J/mol×K	1043.59	Joback Method
cpg	770.26	J/mol×K	1082.83	Joback Method
cpg	777.35	J/mol×K	1122.07	Joback Method
dvisc	0.0004361	Pa×s	538.41	Joback Method

dvisc	0.0002536	Pa×s	596.45	Joback Method
dvisc	0.0001624	Pa×s	654.48	Joback Method
dvisc	0.0001118	Pa×s	712.52	Joback Method
dvisc	0.0000814	Pa×s	770.56	Joback Method
dvisc	0.0000620	Pa×s	828.59	Joback Method
dvisc	0.0000489	Pa×s	886.63	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=U405670&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