Fumaric acid, 1-phenylprop-1-yl 3-chlorophenyl ester

Inchi: InChI=1S/C19H17ClO4/c1-2-17(14-7-4-3-5-8-14)24-19(22)12-11-18(21)23-16-10-6-9-15(

InchiKey: OZKKFONCAKORGU-VAWYXSNFSA-N

Formula: C19H17ClO4

SMILES: CCC(OC(=O)C=CC(=O)Oc1cccc(Cl)c1)c1ccccc1

Mol. weight [g/mol]: 344.79

Physical Properties

Property code	Value	Unit	Source
gf	-77.70	kJ/mol	Joback Method
hf	-367.30	kJ/mol	Joback Method
hfus	39.11	kJ/mol	Joback Method
hvap	85.37	kJ/mol	Joback Method
log10ws	-5.35		Crippen Method
logp	4.496		Crippen Method
mcvol	253.870	ml/mol	McGowan Method
pc	1923.67	kPa	Joback Method
rinpol	2525.00		NIST Webbook
rinpol	2525.00		NIST Webbook
tb	886.19	K	Joback Method
tc	1124.98	K	Joback Method
tf	523.41	K	Joback Method
vc	0.955	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	720.33	J/mol×K	886.19	Joback Method
cpg	771.04	J/mol×K	1085.18	Joback Method
cpg	763.07	J/mol×K	1045.39	Joback Method
cpg	754.08	J/mol×K	1005.59	Joback Method
cpg	744.00	J/mol×K	965.79	Joback Method
cpg	732.77	J/mol×K	925.99	Joback Method
cpg	778.06	J/mol×K	1124.98	Joback Method
dvisc	0.0000447	Pa×s	886.19	Joback Method

dvisc	0.0000575	Pa×s	825.73	Joback Method
dvisc	0.0000769	Pa×s	765.26	Joback Method
dvisc	0.0001080	Pa×s	704.80	Joback Method
dvisc	0.0001619	Pa×s	644.34	Joback Method
dvisc	0.0002637	Pa×s	583.87	Joback Method
dvisc	0.0004810	Pa×s	523.41	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405903&Units=SI

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