Fumaric acid, 1-phenylprop-1-yl 2,4,6-trichlorophenyl ester

Inchi: InChI=1S/C19H15Cl3O4/c1-2-16(12-6-4-3-5-7-12)25-17(23)8-9-18(24)26-19-14(21)10-13

InchiKey: YLMWLFUPPNSIHN-CMDGGOBGSA-N

Formula: C19H15Cl3O4

SMILES: CCC(OC(=O)C=CC(=O)Oc1c(Cl)cc(Cl)cc1Cl)c1ccccc1

Mol. weight [g/mol]: 413.68

Physical Properties

Property code	Value	Unit	Source
gf	-120.82	kJ/mol	Joback Method
hf	-421.72	kJ/mol	Joback Method
hfus	46.72	kJ/mol	Joback Method
hvap	95.46	kJ/mol	Joback Method
log10ws	-6.72		Crippen Method
logp	5.803		Crippen Method
mcvol	278.350	ml/mol	McGowan Method
pc	1759.49	kPa	Joback Method
rinpol	2771.00		NIST Webbook
rinpol	2771.00		NIST Webbook
tb	971.01	K	Joback Method
tc	1216.87	K	Joback Method
tf	608.29	K	Joback Method
vc	1.052	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	756.26	J/mol×K	971.01	Joback Method
cpg	793.45	J/mol×K	1175.90	Joback Method
cpg	788.09	J/mol×K	1134.92	Joback Method
cpg	781.74	J/mol×K	1093.94	Joback Method
cpg	774.36	J/mol×K	1052.96	Joback Method
cpg	765.89	J/mol×K	1011.99	Joback Method
cpg	797.89	J/mol×K	1216.87	Joback Method
dvisc	0.0000341	Pa×s	971.01	Joback Method

dvisc	0.0000427	Pa×s	910.56	Joback Method
dvisc	0.0000552	Pa×s	850.10	Joback Method
dvisc	0.0000741	Pa×s	789.65	Joback Method
dvisc	0.0001046	Pa×s	729.20	Joback Method
dvisc	0.0001570	Pa×s	668.74	Joback Method
dvisc	0.0002555	Pa×s	608.29	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405906&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

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