Fumaric acid, 2-chlorophenyl 2,4,6-trichlorophenyl ester

Inchi: InChI=1S/C16H8Cl4O4/c17-9-7-11(19)16(12(20)8-9)24-15(22)6-5-14(21)23-13-4-2-1-3-1

InchiKey: PSKIHICXNAWKPY-AATRIKPKSA-N

Formula: C16H8Cl4O4

SMILES: O=C(C=CC(=O)Oc1c(Cl)cc(Cl)cc1Cl)Oc1ccccc1Cl

Mol. weight [g/mol]: 406.04

Physical Properties

Property code	Value	Unit	Source
gf	-165.20	kJ/mol	Joback Method
hf	-381.73	kJ/mol	Joback Method
hfus	46.29	kJ/mol	Joback Method
hvap	94.22	kJ/mol	Joback Method
log10ws	-6.34		Crippen Method
logp	5.367		Crippen Method
mcvol	248.320	ml/mol	McGowan Method
pc	2151.31	kPa	Joback Method
rinpol	2735.00		NIST Webbook
rinpol	2735.00		NIST Webbook
tb	945.22	K	Joback Method
tc	1199.71	K	Joback Method
tf	631.92	K	Joback Method
vc	0.940	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	603.57	J/mol×K	945.22	Joback Method
cpg	611.11	J/mol×K	987.64	Joback Method
cpg	617.60	J/mol×K	1030.05	Joback Method
cpg	623.09	J/mol×K	1072.47	Joback Method
cpg	627.60	J/mol×K	1114.88	Joback Method
cpg	631.19	J/mol×K	1157.30	Joback Method
cpg	633.89	J/mol×K	1199.71	Joback Method
dvisc	0.0002539	Pa×s	631.92	Joback Method

dvisc	0.0001751	Pa×s	684.14	Joback Method
dvisc	0.0001273	Pa×s	736.35	Joback Method
dvisc	0.0000965	Pa×s	788.57	Joback Method
dvisc	0.0000758	Pa×s	840.79	Joback Method
dvisc	0.0000612	Pa×s	893.00	Joback Method
dvisc	0.0000506	Pa×s	945.22	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=U405728&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