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

Inchi: InChI=1S/C16H7Cl5O4/c17-8-6-11(20)16(12(21)7-8)25-14(23)5-4-13(22)24-15-9(18)2-1-

InchiKey: VVSLIWPWPNEULH-SNAWJCMRSA-N

Formula: C16H7Cl5O4

SMILES: O=C(C=CC(=O)Oc1c(Cl)cc(Cl)cc1Cl)Oc1c(Cl)cccc1Cl

Mol. weight [g/mol]: 440.49

Physical Properties

Property code	Value	Unit	Source
gf	-186.76	kJ/mol	Joback Method
hf	-408.94	kJ/mol	Joback Method
hfus	50.09	kJ/mol	Joback Method
hvap	99.27	kJ/mol	Joback Method
log10ws	-7.03		Crippen Method
logp	6.021		Crippen Method
mcvol	260.560	ml/mol	McGowan Method
pc	2051.17	kPa	Joback Method
rinpol	2906.00		NIST Webbook
rinpol	2906.00		NIST Webbook
tb	987.63	K	Joback Method
tc	1245.05	K	Joback Method
tf	674.36	K	Joback Method
vc	0.989	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	616.43	J/mol×K	987.63	Joback Method
cpg	622.68	J/mol×K	1030.53	Joback Method
cpg	627.90	J/mol×K	1073.44	Joback Method
cpg	632.10	J/mol×K	1116.34	Joback Method
cpg	635.34	J/mol×K	1159.24	Joback Method
cpg	637.63	J/mol×K	1202.15	Joback Method
cpg	639.02	J/mol×K	1245.05	Joback Method
dvisc	0.0001984	Pa×s	674.36	Joback Method

dvisc	0.0001411	Pa×s	726.57	Joback Method
dvisc	0.0001051	Pa×s	778.78	Joback Method
dvisc	0.0000812	Pa×s	831.00	Joback Method
dvisc	0.0000647	Pa×s	883.21	Joback Method
dvisc	0.0000528	Pa×s	935.42	Joback Method
dvisc	0.0000441	Pa×s	987.63	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=U405865&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