Fumaric acid, 2,4-dichlorophenyl 2-chloro-6-fluorophenyl ester

Inchi: InChI=1S/C16H8Cl3FO4/c17-9-4-5-13(11(19)8-9)23-14(21)6-7-15(22)24-16-10(18)2-1-3-

InchiKey: WXIBSFVSPWHGSG-VOTSOKGWSA-N

Formula: C16H8Cl3FO4

SMILES: O=C(C=CC(=O)Oc1c(F)cccc1Cl)Oc1ccc(Cl)cc1Cl

Mol. weight [g/mol]: 389.59

Physical Properties

Property code	Value	Unit	Source
gf	-348.08	kJ/mol	Joback Method
hf	-562.10	kJ/mol	Joback Method
hfus	45.17	kJ/mol	Joback Method
hvap	89.02	kJ/mol	Joback Method
log10ws	-5.99		Crippen Method
logp	4.853		Crippen Method
mcvol	237.850	ml/mol	McGowan Method
pc	2135.43	kPa	Joback Method
rinpol	2589.00		NIST Webbook
rinpol	2589.00		NIST Webbook
tb	907.06	K	Joback Method
tc	1150.98	K	Joback Method
tf	602.59	K	Joback Method
vc	0.908	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	594.35	J/mol×K	907.06	Joback Method
cpg	602.68	J/mol×K	947.71	Joback Method
cpg	610.00	J/mol×K	988.37	Joback Method
cpg	616.33	J/mol×K	1029.02	Joback Method
cpg	621.72	J/mol×K	1069.67	Joback Method
cpg	626.19	J/mol×K	1110.33	Joback Method
cpg	629.78	J/mol×K	1150.98	Joback Method

Sources

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=U405700&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
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