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

Inchi: InChI=1S/C16H9Cl2FO4/c17-10-4-3-5-11(18)16(10)23-15(21)9-8-14(20)22-13-7-2-1-6-12

InchiKey: KKYPBSRWJNKHBH-CMDGGOBGSA-N

Formula: C16H9Cl2FO4

SMILES: O=C(C=CC(=O)Oc1c(Cl)cccc1Cl)Oc1ccccc1F

Mol. weight [g/mol]: 355.14

Physical Properties

Property code	Value	Unit	Source
gf	-326.52	kJ/mol	Joback Method
hf	-534.89	kJ/mol	Joback Method
hfus	41.36	kJ/mol	Joback Method
hvap	83.97	kJ/mol	Joback Method
log10ws	-5.30		Crippen Method
logp	4.200		Crippen Method
mcvol	225.610	ml/mol	McGowan Method
pc	2241.88	kPa	Joback Method
rinpol	2427.00		NIST Webbook
rinpol	2427.00		NIST Webbook
tb	864.65	K	Joback Method
tc	1105.45	K	Joback Method
tf	560.15	K	Joback Method
vc	0.860	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	578.33	J/mol×K	864.65	Joback Method
cpg	587.94	J/mol×K	904.78	Joback Method
cpg	596.52	J/mol×K	944.92	Joback Method
cpg	604.10	J/mol×K	985.05	Joback Method
cpg	610.73	J/mol×K	1025.18	Joback Method
cpg	616.43	J/mol×K	1065.31	Joback Method
cpg	621.25	J/mol×K	1105.45	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=U405862&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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