Fumaric acid, 2-methoxyphenyl 2-chloro-6-fluorophenyl ester

Inchi: InChI=1S/C17H12ClFO5/c1-22-13-7-2-3-8-14(13)23-15(20)9-10-16(21)24-17-11(18)5-4-6

InchiKey: RDMGWPMUSIDURH-MDZDMXLPSA-N

Formula: C17H12ClFO5

SMILES: COc1ccccc1OC(=O)C=CC(=O)Oc1c(F)cccc1Cl

Mol. weight [g/mol]: 350.73

Physical Properties

Property code	Value	Unit	Source
gf	-411.17	kJ/mol	Joback Method
hf	-672.01	kJ/mol	Joback Method
hfus	40.94	kJ/mol	Joback Method
hvap	84.22	kJ/mol	Joback Method
log10ws	-4.74		Crippen Method
logp	3.555		Crippen Method
mcvol	233.330	ml/mol	McGowan Method
pc	2088.84	kPa	Joback Method
rinpol	2470.00		NIST Webbook
rinpol	2470.00		NIST Webbook
tb	872.52	K	Joback Method
tc	1105.37	K	Joback Method
tf	563.73	K	Joback Method
vc	0.884	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	637.97	J/mol×K	872.52	Joback Method
cpg	648.58	J/mol×K	911.33	Joback Method
cpg	658.03	J/mol×K	950.14	Joback Method
cpg	666.34	J/mol×K	988.94	Joback Method
cpg	673.52	J/mol×K	1027.75	Joback Method
cpg	679.60	J/mol×K	1066.56	Joback Method
cpg	684.59	J/mol×K	1105.37	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405936&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
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