Fumaric acid, 3,5-dimethylphenyl 2-chloro-6-fluorophenyl ester

Inchi: InChI=1S/C18H14ClFO4/c1-11-8-12(2)10-13(9-11)23-16(21)6-7-17(22)24-18-14(19)4-3-5

InchiKey: QOXDHJNNPDWUNT-VOTSOKGWSA-N

Formula: C18H14ClFO4

SMILES: Cc1cc(C)cc(OC(=O)C=CC(=O)Oc2c(F)cccc2Cl)c1

Mol. weight [g/mol]: 348.75

Physical Properties

Property code	Value	Unit	Source
gf	-307.38	kJ/mol	Joback Method
hf	-571.90	kJ/mol	Joback Method
hfus	41.96	kJ/mol	Joback Method
hvap	84.70	kJ/mol	Joback Method
log10ws	-5.57		Crippen Method
logp	4.163		Crippen Method
mcvol	241.550	ml/mol	McGowan Method
pc	1920.30	kPa	Joback Method
rinpol	2486.00		NIST Webbook
rinpol	2486.00		NIST Webbook
tb	877.96	K	Joback Method
tc	1110.69	K	Joback Method
tf	565.29	K	Joback Method
vc	0.922	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	666.56	J/mol×K	877.96	Joback Method
cpg	677.90	J/mol×K	916.75	Joback Method
cpg	688.14	J/mol×K	955.54	Joback Method
cpg	697.30	J/mol×K	994.32	Joback Method
cpg	705.42	J/mol×K	1033.11	Joback Method
cpg	712.53	J/mol×K	1071.90	Joback Method
cpg	718.66	J/mol×K	1110.69	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=U405742&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