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

Inchi: InChI=1S/C17H9ClFNO4/c18-13-2-1-3-14(19)17(13)24-16(22)9-8-15(21)23-12-6-4-11(10

InchiKey: JHZNSHPFGRZTTI-CMDGGOBGSA-N

Formula: C17H9ClFNO4

SMILES: N#Cc1ccc(OC(=O)C=CC(=O)Oc2c(F)cccc2Cl)cc1

Mol. weight [g/mol]: 345.71

Physical Properties

Property code	Value	Unit	Source
gf	-172.99	kJ/mol	Joback Method
hf	-374.91	kJ/mol	Joback Method
hfus	41.26	kJ/mol	Joback Method
hvap	92.29	kJ/mol	Joback Method
log10ws	-4.97		Crippen Method
logp	3.418		Crippen Method
mcvol	228.840	ml/mol	McGowan Method
pc	2073.65	kPa	Joback Method
rinpol	2666.00		NIST Webbook
rinpol	2666.00		NIST Webbook
tb	952.18	K	Joback Method
tc	1197.41	K	Joback Method
tf	606.49	K	Joback Method
vc	0.892	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	617.41	J/mol×K	952.18	Joback Method
cpg	625.25	J/mol×K	993.05	Joback Method
cpg	632.06	J/mol×K	1033.92	Joback Method
cpg	637.88	J/mol×K	1074.80	Joback Method
cpg	642.75	J/mol×K	1115.67	Joback Method
cpg	646.71	J/mol×K	1156.54	Joback Method
cpg	649.79	J/mol×K	1197.41	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=U405733&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