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

Inchi: InChI=1S/C18H22ClFO4/c1-12(10-18(2,3)4)11-23-15(21)8-9-16(22)24-17-13(19)6-5-7-14

InchiKey: ZICUXANOGIGFLX-CMDGGOBGSA-N

Formula: C18H22ClFO4

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

Mol. weight [g/mol]: 356.82

Physical Properties

Property code	Value	Unit	Source
gf	-400.13	kJ/mol	Joback Method
hf	-799.52	kJ/mol	Joback Method
hfus	37.76	kJ/mol	Joback Method
hvap	79.42	kJ/mol	Joback Method
log10ws	-5.22		Crippen Method
logp	4.556		Crippen Method
mcvol	265.310	ml/mol	McGowan Method
pc	1530.66	kPa	Joback Method
rinpol	2226.00		NIST Webbook
rinpol	2226.00		NIST Webbook
tb	837.65	K	Joback Method
tc	1050.99	K	Joback Method
tf	501.25	K	Joback Method
vc	1.014	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	770.12	J/mol×K	837.65	Joback Method
cpg	783.93	J/mol×K	873.21	Joback Method
cpg	796.71	J/mol×K	908.76	Joback Method
cpg	808.52	J/mol×K	944.32	Joback Method
cpg	819.40	J/mol×K	979.88	Joback Method
cpg	829.40	J/mol×K	1015.43	Joback Method
cpg	838.58	J/mol×K	1050.99	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405609&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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