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

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

InchiKey: PWUGCMCFYJGEIY-VAWYXSNFSA-N

Formula: C18H22ClFO4

SMILES: CCCCCCC(C)OC(=O)C=CC(=O)Oc1c(F)cccc1Cl

Mol. weight [g/mol]: 356.82

Physical Properties

Property code	Value	Unit	Source
gf	-402.97	kJ/mol	Joback Method
hf	-790.77	kJ/mol	Joback Method
hfus	45.17	kJ/mol	Joback Method
hvap	80.71	kJ/mol	Joback Method
log10ws	-5.82		Crippen Method
logp	4.843		Crippen Method
mcvol	265.310	ml/mol	McGowan Method
pc	1508.15	kPa	Joback Method
rinpol	2289.00		NIST Webbook
rinpol	2289.00		NIST Webbook
tb	840.88	K	Joback Method
tc	1047.60	K	Joback Method
tf	498.83	K	Joback Method
vc	1.024	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	768.80	J/mol×K	840.88	Joback Method
cpg	782.46	J/mol×K	875.33	Joback Method
cpg	795.11	J/mol×K	909.79	Joback Method
cpg	806.79	J/mol×K	944.24	Joback Method
cpg	817.52	J/mol×K	978.70	Joback Method
cpg	827.33	J/mol×K	1013.15	Joback Method
cpg	836.26	J/mol×K	1047.60	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=U405589&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