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

Inchi: InChI=1S/C16H18ClFO4/c1-3-5-11(2)10-21-14(19)8-9-15(20)22-16-12(17)6-4-7-13(16)18

InchiKey: RGXGITCCZOJNIL-CMDGGOBGSA-N

Formula: C16H18ClFO4

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

Mol. weight [g/mol]: 328.76

Physical Properties

Property code	Value	Unit	Source
gf	-419.81	kJ/mol	Joback Method
hf	-749.49	kJ/mol	Joback Method
hfus	39.99	kJ/mol	Joback Method
hvap	76.26	kJ/mol	Joback Method
log10ws	-4.63		Crippen Method
logp	3.920		Crippen Method
mcvol	237.130	ml/mol	McGowan Method
pc	1760.97	kPa	Joback Method
rinpol	2124.00		NIST Webbook
rinpol	2124.00		NIST Webbook
tb	795.12	K	Joback Method
tc	1003.62	K	Joback Method
tf	476.29	K	Joback Method
vc	0.912	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	656.64	J/mol×K	795.12	Joback Method
cpg	669.69	J/mol×K	829.87	Joback Method
cpg	681.81	J/mol×K	864.62	Joback Method
cpg	693.01	J/mol×K	899.37	Joback Method
cpg	703.33	J/mol×K	934.12	Joback Method
cpg	712.77	J/mol×K	968.87	Joback Method
cpg	721.37	J/mol×K	1003.62	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=U405649&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