Fumaric acid, 3-chlorophenyl 2-fluorophenyl ester

Inchi: InChI=1S/C16H10ClFO4/c17-11-4-3-5-12(10-11)21-15(19)8-9-16(20)22-14-7-2-1-6-13(14

InchiKey: OWTFDJDNPSLJIH-CMDGGOBGSA-N

Formula: C16H10ClFO4

SMILES: O=C(C=CC(=O)Oc1ccccc1F)Oc1cccc(Cl)c1

Mol. weight [g/mol]: 320.70

Physical Properties

Property code	Value	Unit	Source
gf	-304.96	kJ/mol	Joback Method
hf	-507.68	kJ/mol	Joback Method
hfus	37.55	kJ/mol	Joback Method
hvap	78.92	kJ/mol	Joback Method
log10ws	-4.62		Crippen Method
logp	3.546		Crippen Method
mcvol	213.370	ml/mol	McGowan Method
pc	2356.49	kPa	Joback Method
rinpol	2322.00		NIST Webbook
rinpol	2322.00		NIST Webbook
tb	822.24	K	Joback Method
tc	1059.97	K	Joback Method
tf	517.71	K	Joback Method
vc	0.810	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	560.45	J/mol×K	822.24	Joback Method
cpg	571.39	J/mol×K	861.86	Joback Method
cpg	581.25	J/mol×K	901.48	Joback Method
cpg	590.10	J/mol×K	941.11	Joback Method
cpg	597.97	J/mol×K	980.73	Joback Method
cpg	604.89	J/mol×K	1020.35	Joback Method
cpg	610.93	J/mol×K	1059.97	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=U405852&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