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

Inchi: InChI=1S/C16H9ClFNO6/c17-10-4-3-5-11(18)16(10)25-15(21)9-8-14(20)24-13-7-2-1-6-1

InchiKey: OVJSILMFDDUUBF-CMDGGOBGSA-N

Formula: C16H9ClFNO6

SMILES: O=C(C=CC(=O)Oc1c(F)cccc1Cl)Oc1ccccc1[N+](=O)[O-]

Mol. weight [g/mol]: 365.70

Physical Properties

Property code	Value	Unit	Source
gf	-279.04	kJ/mol	Joback Method
hf	-529.91	kJ/mol	Joback Method
hfus	48.52	kJ/mol	Joback Method
hvap	96.18	kJ/mol	Joback Method
log10ws	-5.27		Crippen Method
logp	3.454		Crippen Method
mcvol	230.790	ml/mol	McGowan Method
pc	2349.64	kPa	Joback Method
rinpol	2656.00		NIST Webbook
tb	979.06	K	Joback Method
tc	1233.96	K	Joback Method
tf	673.84	K	Joback Method
vc	0.892	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	640.79	J/mol×K	979.06	Joback Method
cpg	648.31	J/mol×K	1021.54	Joback Method
cpg	654.69	J/mol×K	1064.03	Joback Method
cpg	660.01	J/mol×K	1106.51	Joback Method
cpg	664.30	J/mol×K	1148.99	Joback Method
cpg	667.61	J/mol×K	1191.48	Joback Method
cpg	670.01	J/mol×K	1233.96	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405798&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

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