Fumaric acid, 2-nitrophenyl 2-fluorophenyl ester

Inchi: InChI=1S/C16H10FNO6/c17-11-5-1-3-7-13(11)23-15(19)9-10-16(20)24-14-8-4-2-6-12(14

InchiKey: WCIGVJVDAZONMQ-MDZDMXLPSA-N

Formula: C16H10FNO6

SMILES: O=C(C=CC(=O)Oc1ccccc1[N+](=O)[O-])Oc1ccccc1F

Mol. weight [g/mol]: 331.25

Physical Properties

Property code	Value	Unit	Source
gf	-257.48	kJ/mol	Joback Method
hf	-502.70	kJ/mol	Joback Method
hfus	44.72	kJ/mol	Joback Method
hvap	91.13	kJ/mol	Joback Method
log10ws	-4.58		Crippen Method
logp	2.801		Crippen Method
mcvol	218.550	ml/mol	McGowan Method
pc	2472.73	kPa	Joback Method
rinpol	2519.00		NIST Webbook
rinpol	2519.00		NIST Webbook
tb	936.65	K	Joback Method
tc	1188.53	K	Joback Method
tf	631.40	K	Joback Method
vc	0.844	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	626.44	J/mol×K	936.65	Joback Method
cpg	635.33	J/mol×K	978.63	Joback Method
cpg	643.07	J/mol×K	1020.61	Joback Method
cpg	649.72	J/mol×K	1062.59	Joback Method
cpg	655.33	J/mol×K	1104.57	Joback Method
cpg	659.96	J/mol×K	1146.55	Joback Method
cpg	663.67	J/mol×K	1188.53	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405795&Units=SI

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