Fumaric acid, 2-nitrophenyl 3-chlorophenyl ester

Inchi: InChI=1S/C16H10ClNO6/c17-11-4-3-5-12(10-11)23-15(19)8-9-16(20)24-14-7-2-1-6-13(1
InchiKey: BGDUJOFVJOVGRP-CMDGGOBGSA-N
Formula: C16H10ClNO6
SMILES: O=C(C=CC(=O)Oc1ccccc1[N+](=O)[O-])Oc1cccc(Cl)c1
Mol. weight [g/mol]: 347.71

Physical Properties

Property code	Value	Unit	Source
gf	-74.60	kJ/mol	Joback Method
hf	-322.33	kJ/mol	Joback Method
hfus	45.83	kJ/mol	Joback Method
hvap	96.33	kJ/mol	Joback Method
log10ws	-4.94		Crippen Method
logp	3.315		Crippen Method
mcvol	229.020	ml/mol	McGowan Method
pc	2492.52	kPa	Joback Method
rinpol	2709.00		NIST Webbook
tb	974.81	K	Joback Method
tc	1237.27	K	Joback Method
tf	660.73	K	Joback Method
vc	0.875	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	635.84	J/mol×K	974.81	Joback Method
cpg	643.87	J/mol×K	1018.55	Joback Method
cpg	650.73	J/mol×K	1062.30	Joback Method
cpg	656.49	J/mol×K	1106.04	Joback Method
cpg	661.21	J/mol×K	1149.78	Joback Method
cpg	664.97	J/mol×K	1193.53	Joback Method
cpg	667.82	J/mol×K	1237.27	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=U405799&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