Fumaric acid, 2-nitrophenyl 2,3-dichlorophenyl ester

Inchi: InChI=1S/C16H9Cl2NO6/c17-10-4-3-7-13(16(10)18)25-15(21)9-8-14(20)24-12-6-2-1-5-1

InchiKey: XACSXBHSFQCUCT-CMDGGOBGSA-N

Formula: C16H9Cl2NO6

SMILES: O=C(C=CC(=O)Oc1cccc(Cl)c1Cl)Oc1ccccc1[N+](=O)[O-]

Mol. weight [g/mol]: 382.15

Physical Properties

Property code	Value	Unit	Source
gf	-96.16	kJ/mol	Joback Method
hf	-349.54	kJ/mol	Joback Method
hfus	49.64	kJ/mol	Joback Method
hvap	101.38	kJ/mol	Joback Method
log10ws	-5.62		Crippen Method
logp	3.969		Crippen Method
mcvol	241.260	ml/mol	McGowan Method
pc	2367.97	kPa	Joback Method
rinpol	2925.00		NIST Webbook
rinpol	2925.00		NIST Webbook
tb	1017.22	K	Joback Method
tc	1282.35	K	Joback Method
tf	703.17	K	Joback Method
vc	0.923	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	648.75	J/mol×K	1017.22	Joback Method
cpg	655.38	J/mol×K	1061.41	Joback Method
cpg	660.88	J/mol×K	1105.60	Joback Method
cpg	665.30	J/mol×K	1149.79	Joback Method
cpg	668.69	J/mol×K	1193.98	Joback Method
cpg	671.12	J/mol×K	1238.17	Joback Method
cpg	672.65	J/mol×K	1282.35	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=U405801&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