Fumaric acid, 4-cyanophenyl 3-chlorophenyl ester

Inchi: InChI=1S/C17H10ClNO4/c18-13-2-1-3-15(10-13)23-17(21)9-8-16(20)22-14-6-4-12(11-19

InchiKey: UBZWUVWISGRVPC-CMDGGOBGSA-N

Formula: C17H10ClNO4

SMILES: N#Cc1ccc(OC(=O)C=CC(=O)Oc2cccc(Cl)c2)cc1

Mol. weight [g/mol]: 327.72

Physical Properties

Property code	Value	Unit	Source
gf	31.45	kJ/mol	Joback Method
hf	-167.33	kJ/mol	Joback Method
hfus	38.57	kJ/mol	Joback Method
hvap	92.45	kJ/mol	Joback Method
log10ws	-4.64		Crippen Method
logp	3.279		Crippen Method
mcvol	227.070	ml/mol	McGowan Method
pc	2191.78	kPa	Joback Method
rinpol	3175.00		NIST Webbook
rinpol	3175.00		NIST Webbook
tb	947.93	K	Joback Method
tc	1200.15	K	Joback Method
tf	593.38	K	Joback Method
vc	0.875	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	612.30	J/mol×K	947.93	Joback Method
cpg	620.62	J/mol×K	989.97	Joback Method
cpg	627.88	J/mol×K	1032.00	Joback Method
cpg	634.12	J/mol×K	1074.04	Joback Method
cpg	639.39	J/mol×K	1116.07	Joback Method
cpg	643.75	J/mol×K	1158.11	Joback Method
cpg	647.24	J/mol×K	1200.15	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405734&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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