Succinic acid, 4-cyanophenyl 2,3-dichlorophenyl ester

Inchi: InChI=1S/C17H11Cl2NO4/c18-13-2-1-3-14(17(13)19)24-16(22)9-8-15(21)23-12-6-4-11(1

InchiKey: PKDWSBSDCSHHAB-UHFFFAOYSA-N

Formula: C17H11Cl2NO4

SMILES: N#Cc1ccc(OC(=O)CCC(=O)Oc2cccc(Cl)c2Cl)cc1

Mol. weight [g/mol]: 364.18

Physical Properties

Property code	Value	Unit	Source
gf	-70.33	kJ/mol	Joback Method
hf	-311.76	kJ/mol	Joback Method
hfus	42.17	kJ/mol	Joback Method
hvap	97.53	kJ/mol	Joback Method
log10ws	-5.47		Crippen Method
logp	4.156		Crippen Method
mcvol	243.610	ml/mol	McGowan Method
pc	1992.98	kPa	Joback Method
rinpol	2962.00		NIST Webbook
tb	986.18	K	Joback Method
tc	1235.17	K	Joback Method
tf	640.90	K	Joback Method
vc	0.944	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	655.74	J/mol×K	986.18	Joback Method
cpg	662.90	J/mol×K	1027.68	Joback Method
cpg	668.84	J/mol×K	1069.18	Joback Method
cpg	673.57	J/mol×K	1110.67	Joback Method
cpg	677.14	J/mol×K	1152.17	Joback Method
cpg	679.55	J/mol×K	1193.67	Joback Method
cpg	680.83	J/mol×K	1235.17	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=U360709&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