Succinic acid, 4-chloro-3-methylphenyl 2,4,6-trichlorophenyl ester

Inchi: InChI=1S/C17H12Cl4O4/c1-9-6-11(2-3-12(9)19)24-15(22)4-5-16(23)25-17-13(20)7-10(18)8-14(17)21/h2-3,6-8H,4-5H2,1H3

InchiKey: AKBPTYDLNXKJNG-UHFFFAOYSA-N

Formula: C17H12Cl4O4

SMILES: Cc1cc(OC(=O)CCC(=O)Oc2c(Cl)cc(Cl)cc2Cl)ccc1Cl

Mol. weight [g/mol]: 422.09

Physical Properties

Property code	Value	Unit	Source
gf	-246.63	kJ/mol	Joback Method
hf	-531.06	kJ/mol	Joback Method
hfus	48.29	kJ/mol	Joback Method
hvap	97.15	kJ/mol	Joback Method
log10ws	-6.96		Crippen Method
logp	5.900		Crippen Method
mcvol	266.710	ml/mol	McGowan Method
pc	1859.51	kPa	Joback Method
rinpol	2897.00		NIST Webbook
rinpol	2897.00		NIST Webbook
tb	968.92	K	Joback Method
tc	1214.51	K	Joback Method
tf	660.79	K	Joback Method
vc	1.016	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	686.12	J/mol×K	968.92	Joback Method
cpg	694.03	J/mol×K	1009.85	Joback Method
cpg	700.69	J/mol×K	1050.78	Joback Method
cpg	706.12	J/mol×K	1091.71	Joback Method
cpg	710.32	J/mol×K	1132.64	Joback Method
cpg	713.31	J/mol×K	1173.57	Joback Method
cpg	715.10	J/mol×K	1214.51	Joback Method
dvisc	0.0002316	Pa×s	660.79	Joback Method

dvisc	0.0001643	Pa×s	712.15	Joback Method
dvisc	0.0001221	Pa×s	763.50	Joback Method
dvisc	0.0000942	Pa×s	814.86	Joback Method
dvisc	0.0000749	Pa×s	866.21	Joback Method
dvisc	0.0000612	Pa×s	917.57	Joback Method
dvisc	0.0000510	Pa×s	968.92	Joback Method

Sources

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=U390282&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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