Succinic acid, 3-chlorophenyl 2,6-dichlorophenyl ester

Inchi: InChI=1S/C16H11Cl3O4/c17-10-3-1-4-11(9-10)22-14(20)7-8-15(21)23-16-12(18)5-2-6-13

InchiKey: KHUUMWCBFLAHFG-UHFFFAOYSA-N

Formula: C16H11Cl3O4

SMILES: O=C(CCC(=O)Oc1c(Cl)cccc1Cl)Oc1cccc(Cl)c1

Mol. weight [g/mol]: 373.62

Physical Properties

Property code	Value	Unit	Source
gf	-223.86	kJ/mol	Joback Method
hf	-471.74	kJ/mol	Joback Method
hfus	42.28	kJ/mol	Joback Method
hvap	89.21	kJ/mol	Joback Method
log10ws	-5.80		Crippen Method
logp	4.938		Crippen Method
mcvol	240.380	ml/mol	McGowan Method
pc	2151.31	kPa	Joback Method
rinpol	2717.00		NIST Webbook
rinpol	2717.00		NIST Webbook
tb	898.65	K	Joback Method
tc	1142.90	K	Joback Method
tf	594.56	K	Joback Method
vc	0.910	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	617.57	J/mol×K	898.65	Joback Method
cpg	652.35	J/mol×K	1102.20	Joback Method
cpg	647.66	J/mol×K	1061.49	Joback Method
cpg	641.86	J/mol×K	1020.78	Joback Method
cpg	634.92	J/mol×K	980.07	Joback Method
cpg	626.83	J/mol×K	939.36	Joback Method
cpg	655.95	J/mol×K	1142.90	Joback Method
dvisc	0.0000659	Pa×s	898.65	Joback Method

dvisc	0.0000803	Pa×s	847.97	Joback Method
dvisc	0.0001004	Pa×s	797.29	Joback Method
dvisc	0.0001294	Pa×s	746.61	Joback Method
dvisc	0.0001731	Pa×s	695.92	Joback Method
dvisc	0.0002423	Pa×s	645.24	Joback Method
dvisc	0.0003592	Pa×s	594.56	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U389870&Units=SI

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