Succinic acid, 2,3-dichlorophenyl 2,4,5-trichlorophenyl ester

Inchi: InChI=1S/C16H9Cl5O4/c17-8-2-1-3-12(16(8)21)24-14(22)4-5-15(23)25-13-7-10(19)9(18)6-11(13)20

InchiKey: XIKZQZRRXIQPNI-UHFFFAOYSA-N

Formula: C16H9Cl5O4

SMILES: O=C(CCC(=O)Oc1cccc(Cl)c1Cl)Oc1cc(Cl)c(Cl)cc1Cl

Mol. weight [g/mol]: 442.50

Physical Properties

Property code	Value	Unit	Source
gf	-266.98	kJ/mol	Joback Method
hf	-526.16	kJ/mol	Joback Method
hfus	49.89	kJ/mol	Joback Method
hvap	99.31	kJ/mol	Joback Method
log10ws	-7.17		Crippen Method
logp	6.245		Crippen Method
mcvol	264.860	ml/mol	McGowan Method
pc	1957.87	kPa	Joback Method
rinpol	3034.00		NIST Webbook
rinpol	3034.00		NIST Webbook
tb	983.47	K	Joback Method
tc	1234.30	K	Joback Method
tf	679.44	K	Joback Method
vc	1.008	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	646.24	J/mol×K	983.47	Joback Method
cpg	652.65	J/mol×K	1025.27	Joback Method
cpg	657.85	J/mol×K	1067.08	Joback Method
cpg	661.86	J/mol×K	1108.88	Joback Method
cpg	664.68	J/mol×K	1150.69	Joback Method
cpg	666.31	J/mol×K	1192.49	Joback Method
cpg	666.79	J/mol×K	1234.30	Joback Method
dvisc	0.0002171	Pa×s	679.44	Joback Method

dvisc	0.0001562	Pa×s	730.11	Joback Method
dvisc	0.0001173	Pa×s	780.78	Joback Method
dvisc	0.0000912	Pa×s	831.46	Joback Method
dvisc	0.0000730	Pa×s	882.13	Joback Method
dvisc	0.0000599	Pa×s	932.80	Joback Method
dvisc	0.0000501	Pa×s	983.47	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=U389974&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