Succinic acid, 2,4,6-trichlorophenyl 2,4,5-trichlorophenyl ester

Inchi: InChI=1S/C16H8Cl6O4/c17-7-3-11(21)16(12(22)4-7)26-15(24)2-1-14(23)25-13-6-9(19)8(

InchiKey: FFMSIBSMKXDCPP-UHFFFAOYSA-N

Formula: C16H8Cl6O4

SMILES: O=C(CCC(=O)Oc1c(Cl)cc(Cl)cc1Cl)Oc1cc(Cl)c(Cl)cc1Cl

Mol. weight [g/mol]: 476.95

Physical Properties

Property code	Value	Unit	Source
gf	-288.54	kJ/mol	Joback Method
hf	-553.37	kJ/mol	Joback Method
hfus	53.70	kJ/mol	Joback Method
hvap	104.36	kJ/mol	Joback Method
log10ws	-7.86		Crippen Method
logp	6.898		Crippen Method
mcvol	277.100	ml/mol	McGowan Method
pc	1870.79	kPa	Joback Method
rinpol	3088.00		NIST Webbook
rinpol	3088.00		NIST Webbook
tb	1025.88	K	Joback Method
tc	1280.42	K	Joback Method
tf	721.88	K	Joback Method
vc	1.058	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	657.78	J/mol×K	1025.88	Joback Method
cpg	662.72	J/mol×K	1068.30	Joback Method
cpg	666.41	J/mol×K	1110.73	Joback Method
cpg	668.86	J/mol×K	1153.15	Joback Method
cpg	670.07	J/mol×K	1195.57	Joback Method
cpg	670.03	J/mol×K	1238.00	Joback Method
cpg	668.76	J/mol×K	1280.42	Joback Method
dvisc	0.0001712	Pa×s	721.88	Joback Method

dvisc	0.0001264	Pa×s	772.55	Joback Method
dvisc	0.0000968	Pa×s	823.21	Joback Method
dvisc	0.0000765	Pa×s	873.88	Joback Method
dvisc	0.0000621	Pa×s	924.55	Joback Method
dvisc	0.0000514	Pa×s	975.21	Joback Method
dvisc	0.0000434	Pa×s	1025.88	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=U389976&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