Succinic acid, 2,4,6-trichlorophenyl 1-phenylpropyl ester

Inchi: InChI=1S/C19H17Cl3O4/c1-2-16(12-6-4-3-5-7-12)25-17(23)8-9-18(24)26-19-14(21)10-13

InchiKey: WXGKPRCZBVQDOG-UHFFFAOYSA-N

Formula: C19H17Cl3O4

SMILES: CCC(OC(=O)CCC(=O)Oc1c(Cl)cc(Cl)cc1Cl)c1ccccc1

Mol. weight [g/mol]: 415.69

Physical Properties

Property code	Value	Unit	Source
gf	-201.04	kJ/mol	Joback Method
hf	-538.94	kJ/mol	Joback Method
hfus	46.52	kJ/mol	Joback Method
hvap	95.50	kJ/mol	Joback Method
log10ws	-6.87		Crippen Method
logp	6.027		Crippen Method
mcvol	282.650	ml/mol	McGowan Method
pc	1685.18	kPa	Joback Method
rinpol	2738.00		NIST Webbook
rinpol	2738.00		NIST Webbook
tb	966.85	K	Joback Method
tc	1206.89	K	Joback Method
tf	613.37	K	Joback Method
vc	1.073	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	785.56	J/mol×K	966.85	Joback Method
cpg	795.36	J/mol×K	1006.86	Joback Method
cpg	803.87	J/mol×K	1046.86	Joback Method
cpg	811.12	J/mol×K	1086.87	Joback Method
cpg	817.15	J/mol×K	1126.88	Joback Method
cpg	821.99	J/mol×K	1166.89	Joback Method
cpg	825.67	J/mol×K	1206.89	Joback Method
dvisc	0.0002781	Pa×s	613.37	Joback Method

dvisc	0.0001735	Pa×s	672.28	Joback Method
dvisc	0.0001168	Pa×s	731.20	Joback Method
dvisc	0.0000834	Pa×s	790.11	Joback Method
dvisc	0.0000624	Pa×s	849.02	Joback Method
dvisc	0.0000485	Pa×s	907.94	Joback Method
dvisc	0.0000389	Pa×s	966.85	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=U389936&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