Succinic acid, ethyl pentachlorophenyl ester

Inchi: InChI=1S/C12H9Cl5O4/c1-2-20-5(18)3-4-6(19)21-12-10(16)8(14)7(13)9(15)11(12)17/h2-
InchiKey: QKWPHHZXXMWGGK-UHFFFAOYSA-N
Formula: C12H9Cl5O4
SMILES: CCOC(=O)CCC(=O)Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl
Mol. weight [g/mol]: 394.46

Physical Properties

Property code	Value	Unit	Source
gf	-413.07	kJ/mol	Joback Method
hf	-680.13	kJ/mol	Joback Method
hfus	45.49	kJ/mol	Joback Method
hvap	88.13	kJ/mol	Joback Method
log10ws	-5.75		Crippen Method
logp	5.202		Crippen Method
mcvol	232.260	ml/mol	McGowan Method
pc	2053.03	kPa	Joback Method
rinpol	2440.00		NIST Webbook
rinpol	2440.00		NIST Webbook
tb	865.27	K	Joback Method
tc	1095.31	K	Joback Method
tf	607.94	K	Joback Method
vc	0.892	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	537.44	J/mol×K	865.27	Joback Method
cpg	545.30	J/mol×K	903.61	Joback Method
cpg	552.27	J/mol×K	941.95	Joback Method
cpg	558.33	J/mol×K	980.29	Joback Method
cpg	563.46	J/mol×K	1018.63	Joback Method
cpg	567.65	J/mol×K	1056.97	Joback Method
cpg	570.88	J/mol×K	1095.31	Joback Method
dvisc	0.0003398	Pa×s	607.94	Joback Method

dvisc	0.0002505	Pa×s	650.83	Joback Method
dvisc	0.0001918	Pa×s	693.72	Joback Method
dvisc	0.0001515	Pa×s	736.61	Joback Method
dvisc	0.0001228	Pa×s	779.49	Joback Method
dvisc	0.0001018	Pa×s	822.38	Joback Method
dvisc	0.0000859	Pa×s	865.27	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=U390051&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