Succinic acid, 2-ethylhexyl pentachlorophenyl ester

Inchi: InChI=1S/C18H21Cl5O4/c1-3-5-6-10(4-2)9-26-11(24)7-8-12(25)27-18-16(22)14(20)13(19

InchiKey: OVNZPJVQRKXMTR-UHFFFAOYSA-N

Formula: C18H21Cl5O4

SMILES: CCCCC(CC)COC(=O)CCC(=O)Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl

Mol. weight [g/mol]: 478.62

Physical Properties

Property code	Value	Unit	Source
gf	-364.99	kJ/mol	Joback Method
hf	-809.25	kJ/mol	Joback Method
hfus	57.51	kJ/mol	Joback Method
hvap	101.10	kJ/mol	Joback Method
log10ws	-8.02		Crippen Method
logp	7.399		Crippen Method
mcvol	316.800	ml/mol	McGowan Method
pc	1298.60	kPa	Joback Method
rinpol	2958.00		NIST Webbook
rinpol	2958.00		NIST Webbook
tb	1002.11	K	Joback Method
tc	1231.88	K	Joback Method
tf	660.56	K	Joback Method
vc	1.222	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	871.72	J/mol×K	1002.11	Joback Method
cpg	905.94	J/mol×K	1193.59	Joback Method
cpg	901.60	J/mol×K	1155.29	Joback Method
cpg	896.02	J/mol×K	1117.00	Joback Method
cpg	889.18	J/mol×K	1078.70	Joback Method
cpg	881.09	J/mol×K	1040.41	Joback Method
cpg	909.04	J/mol×K	1231.88	Joback Method
dvisc	0.0000324	Pa×s	1002.11	Joback Method

dvisc	0.0000397	Pa×s	945.18	Joback Method
dvisc	0.0000501	Pa×s	888.26	Joback Method
dvisc	0.0000651	Pa×s	831.33	Joback Method
dvisc	0.0000881	Pa×s	774.41	Joback Method
dvisc	0.0001249	Pa×s	717.48	Joback Method
dvisc	0.0001883	Pa×s	660.56	Joback Method

Sources

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=U390050&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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