Succinic acid, isobutyl 2,3,5,6-tetrachlorophenyl ester

Inchi: InChI=1S/C14H14Cl4O4/c1-7(2)6-21-10(19)3-4-11(20)22-14-12(17)8(15)5-9(16)13(14)18

InchiKey: HNSFOJLAXWCAGH-UHFFFAOYSA-N

Formula: C14H14Cl4O4

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

Mol. weight [g/mol]: 388.07

Physical Properties

Property code	Value	Unit	Source
gf	-377.11	kJ/mol	Joback Method
hf	-699.48	kJ/mol	Joback Method
hfus	43.34	kJ/mol	Joback Method
hvap	87.15	kJ/mol	Joback Method
log10ws	-5.66		Crippen Method
logp	5.185		Crippen Method
mcvol	248.200	ml/mol	McGowan Method
pc	1827.85	kPa	Joback Method
rinpol	2422.00		NIST Webbook
rinpol	2422.00		NIST Webbook
tb	868.18	K	Joback Method
tc	1092.96	K	Joback Method
tf	573.04	K	Joback Method
vc	0.950	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	629.30	J/mol×K	868.18	Joback Method
cpg	639.17	J/mol×K	905.64	Joback Method
cpg	648.03	J/mol×K	943.11	Joback Method
cpg	655.89	J/mol×K	980.57	Joback Method
cpg	662.75	J/mol×K	1018.04	Joback Method
cpg	668.60	J/mol×K	1055.50	Joback Method
cpg	673.43	J/mol×K	1092.96	Joback Method
dvisc	0.0003825	Pa×s	573.04	Joback Method

dvisc	0.0002558	Pa×s	622.23	Joback Method
dvisc	0.0001814	Pa×s	671.42	Joback Method
dvisc	0.0001349	Pa×s	720.61	Joback Method
dvisc	0.0001041	Pa×s	769.80	Joback Method
dvisc	0.0000829	Pa×s	818.99	Joback Method
dvisc	0.0000678	Pa×s	868.18	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=U353316&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