Succinic acid, 2-isopropoxyphenyl 6-chlorohexyl ester

Inchi: InChI=1S/C19H27ClO5/c1-15(2)24-16-9-5-6-10-17(16)25-19(22)12-11-18(21)23-14-8-4-3

InchiKey: BWPQYVMVSVRIHE-UHFFFAOYSA-N

Formula: C19H27ClO5

SMILES: CC(C)Oc1ccccc1OC(=O)CCC(=O)OCCCCCCCl

Mol. weight [g/mol]: 370.87

Physical Properties

Property code	Value	Unit	Source
gf	-375.33	kJ/mol	Joback Method
hf	-853.27	kJ/mol	Joback Method
hfus	46.05	kJ/mol	Joback Method
hvap	85.54	kJ/mol	Joback Method
log10ws	-5.22		Crippen Method
logp	4.502		Crippen Method
mcvol	287.800	ml/mol	McGowan Method
pc	1392.29	kPa	Joback Method
rinpol	2685.00		NIST Webbook
rinpol	2685.00		NIST Webbook
tb	877.77	K	Joback Method
tc	1085.02	K	Joback Method
tf	524.30	K	Joback Method
vc	1.101	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	875.13	J/mol×K	877.77	Joback Method
cpg	934.60	J/mol×K	1050.48	Joback Method
cpg	925.11	J/mol×K	1015.93	Joback Method
cpg	914.44	J/mol×K	981.39	Joback Method
cpg	902.55	J/mol×K	946.85	Joback Method
cpg	889.46	J/mol×K	912.31	Joback Method
cpg	942.90	J/mol×K	1085.02	Joback Method
dvisc	0.0000373	Pa×s	877.77	Joback Method

dvisc	0.0000483	Pa×s	818.86	Joback Method
dvisc	0.0000650	Pa×s	759.95	Joback Method
dvisc	0.0000921	Pa×s	701.03	Joback Method
dvisc	0.0001391	Pa×s	642.12	Joback Method
dvisc	0.0002283	Pa×s	583.21	Joback Method
dvisc	0.0004188	Pa×s	524.30	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357973&Units=SI
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

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