Succinic acid, 2,2-dichloroethyl 2-isopropoxyphenyl ester

Inchi: InChI=1S/C15H18Cl2O5/c1-10(2)21-11-5-3-4-6-12(11)22-15(19)8-7-14(18)20-9-13(16)17

InchiKey: PZKCIHQYKCDXQT-UHFFFAOYSA-N

Formula: C15H18Cl2O5

SMILES: CC(C)Oc1ccccc1OC(=O)CCC(=O)OCC(Cl)Cl

Mol. weight [g/mol]: 349.21

Physical Properties

Property code	Value	Unit	Source
gf	-423.38	kJ/mol	Joback Method
hf	-791.73	kJ/mol	Joback Method
hfus	36.37	kJ/mol	Joback Method
hvap	80.64	kJ/mol	Joback Method
log10ws	-4.30		Crippen Method
logp	3.506		Crippen Method
mcvol	243.680	ml/mol	McGowan Method
pc	1849.92	kPa	Joback Method
rinpol	2277.00		NIST Webbook
rinpol	2277.00		NIST Webbook
tb	823.24	K	Joback Method
tc	1038.83	K	Joback Method
tf	494.14	K	Joback Method
vc	0.919	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	672.13	J/mol×K	823.24	Joback Method
cpg	684.59	J/mol×K	859.17	Joback Method
cpg	695.94	J/mol×K	895.10	Joback Method
cpg	706.19	J/mol×K	931.03	Joback Method
cpg	715.34	J/mol×K	966.97	Joback Method
cpg	723.39	J/mol×K	1002.90	Joback Method
cpg	730.34	J/mol×K	1038.83	Joback Method
dvisc	0.0005857	Pa×s	494.14	Joback Method

dvisc	0.0003205	Pa×s	548.99	Joback Method
dvisc	0.0001957	Pa×s	603.84	Joback Method
dvisc	0.0001297	Pa×s	658.69	Joback Method
dvisc	0.0000916	Pa×s	713.54	Joback Method
dvisc	0.0000680	Pa×s	768.39	Joback Method
dvisc	0.0000525	Pa×s	823.24	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=U389790&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