Succinic acid, 2-(2-chlorophenoxy)ethyl decyl ester

Inchi: InChI=1S/C22H33ClO5/c1-2-3-4-5-6-7-8-11-16-27-21(24)14-15-22(25)28-18-17-26-20-13

InchiKey: LRWMYIOKGXIBPX-UHFFFAOYSA-N

Formula: C22H33ClO5

SMILES: CCCCCCCCCCOC(=O)CCC(=O)OCCOc1ccccc1Cl

Mol. weight [g/mol]: 412.95

Physical Properties

Property code	Value	Unit	Source
gf	-347.63	kJ/mol	Joback Method
hf	-909.91	kJ/mol	Joback Method
hfus	57.35	kJ/mol	Joback Method
hvap	92.61	kJ/mol	Joback Method
log10ws	-6.28		Crippen Method
logp	5.726		Crippen Method
mcvol	330.070	ml/mol	McGowan Method
pc	1129.10	kPa	Joback Method
rinpol	2943.00		NIST Webbook
rinpol	2943.00		NIST Webbook
tb	946.85	K	Joback Method
tc	1160.06	K	Joback Method
tf	573.11	K	Joback Method
vc	1.274	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1053.04	J/mol×K	946.85	Joback Method
cpg	1067.79	J/mol×K	982.38	Joback Method
cpg	1081.12	J/mol×K	1017.92	Joback Method
cpg	1093.07	J/mol×K	1053.45	Joback Method
cpg	1103.65	J/mol×K	1088.99	Joback Method
cpg	1112.89	J/mol×K	1124.52	Joback Method
cpg	1120.79	J/mol×K	1160.06	Joback Method
dvisc	0.0002696	Pa×s	573.11	Joback Method

dvisc	0.0001509	Pa×s	635.40	Joback Method
dvisc	0.0000937	Pa×s	697.69	Joback Method
dvisc	0.0000629	Pa×s	759.98	Joback Method
dvisc	0.0000448	Pa×s	822.27	Joback Method
dvisc	0.0000335	Pa×s	884.56	Joback Method
dvisc	0.0000260	Pa×s	946.85	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=U381541&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