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

Inchi: InChI=1S/C23H35ClO5/c1-2-3-4-5-6-7-8-9-12-17-28-22(25)15-16-23(26)29-19-18-27-21-

InchiKey: FRHJUJWBUOVXFS-UHFFFAOYSA-N

Formula: C23H35ClO5

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

Mol. weight [g/mol]: 426.97

Physical Properties

Property code	Value	Unit	Source
gf	-339.21	kJ/mol	Joback Method
hf	-930.55	kJ/mol	Joback Method
hfus	59.94	kJ/mol	Joback Method
hvap	94.84	kJ/mol	Joback Method
log10ws	-6.70		Crippen Method
logp	6.116		Crippen Method
mcvol	344.160	ml/mol	McGowan Method
pc	1059.64	kPa	Joback Method
rinpol	3044.00		NIST Webbook
rinpol	3044.00		NIST Webbook
tb	969.73	K	Joback Method
tc	1187.27	K	Joback Method
tf	584.38	K	Joback Method
vc	1.331	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1113.61	J/mol×K	969.73	Joback Method
cpg	1128.52	J/mol×K	1005.99	Joback Method
cpg	1141.93	J/mol×K	1042.24	Joback Method
cpg	1153.87	J/mol×K	1078.50	Joback Method
cpg	1164.36	J/mol×K	1114.75	Joback Method
cpg	1173.42	J/mol×K	1151.01	Joback Method
cpg	1181.08	J/mol×K	1187.27	Joback Method
dvisc	0.0002395	Pa×s	584.38	Joback Method

dvisc	0.0001326	Pa×s	648.61	Joback Method
dvisc	0.0000817	Pa×s	712.83	Joback Method
dvisc	0.0000545	Pa×s	777.06	Joback Method
dvisc	0.0000387	Pa×s	841.28	Joback Method
dvisc	0.0000288	Pa×s	905.50	Joback Method
dvisc	0.0000223	Pa×s	969.73	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=U381542&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

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