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

Inchi: InChI=1S/C29H47ClO5/c1-2-3-4-5-6-7-10-13-18-23-34-28(31)21-14-11-8-9-12-15-22-29(

InchiKey: MDNOKWIULWAYBZ-UHFFFAOYSA-N

Formula: C29H47ClO5

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

Mol. weight [g/mol]: 511.13

Physical Properties

Property code	Value	Unit	Source
gf	-288.69	kJ/mol	Joback Method
hf	-1054.39	kJ/mol	Joback Method
hfus	75.48	kJ/mol	Joback Method
hvap	108.19	kJ/mol	Joback Method
log10ws	-9.21		Crippen Method
logp	8.457		Crippen Method
mcvol	428.700	ml/mol	McGowan Method
pc	751.43	kPa	Joback Method
rinpol	3432.00		NIST Webbook
rinpol	3432.00		NIST Webbook
tb	1107.01	K	Joback Method
tc	1374.89	K	Joback Method
tf	652.00	K	Joback Method
vc	1.667	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1484.65	J/mol×K	1107.01	Joback Method
cpg	1541.43	J/mol×K	1330.24	Joback Method
cpg	1534.61	J/mol×K	1285.60	Joback Method
cpg	1525.60	J/mol×K	1240.95	Joback Method
cpg	1514.33	J/mol×K	1196.30	Joback Method
cpg	1500.71	J/mol×K	1151.66	Joback Method
cpg	1546.16	J/mol×K	1374.89	Joback Method
dvisc	0.0000086	Pa×s	1107.01	Joback Method

dvisc	0.0000113	Pa×s	1031.17	Joback Method
dvisc	0.0000155	Pa×s	955.34	Joback Method
dvisc	0.0000223	Pa×s	879.50	Joback Method
dvisc	0.0000344	Pa×s	803.67	Joback Method
dvisc	0.0000582	Pa×s	727.83	Joback Method
dvisc	0.0001112	Pa×s	652.00	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=U416780&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