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

Inchi: InChI=1S/C27H43ClO5/c1-2-3-4-5-8-11-16-21-32-26(29)19-12-9-6-7-10-13-20-27(30)33-

InchiKey: HTZRYVCQYVAGGJ-UHFFFAOYSA-N

Formula: C27H43ClO5

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

Mol. weight [g/mol]: 483.08

Physical Properties

Property code	Value	Unit	Source
gf	-305.53	kJ/mol	Joback Method
hf	-1013.11	kJ/mol	Joback Method
hfus	70.30	kJ/mol	Joback Method
hvap	103.74	kJ/mol	Joback Method
log10ws	-8.37		Crippen Method
logp	7.677		Crippen Method
mcvol	400.520	ml/mol	McGowan Method
pc	837.24	kPa	Joback Method
rinpol	3229.00		NIST Webbook
rinpol	3229.00		NIST Webbook
tb	1061.25	K	Joback Method
tc	1307.13	K	Joback Method
tf	629.46	K	Joback Method
vc	1.554	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1359.83	J/mol×K	1061.25	Joback Method
cpg	1375.49	J/mol×K	1102.23	Joback Method
cpg	1389.10	J/mol×K	1143.21	Joback Method
cpg	1400.74	J/mol×K	1184.19	Joback Method
cpg	1410.46	J/mol×K	1225.17	Joback Method
cpg	1418.32	J/mol×K	1266.15	Joback Method
cpg	1424.37	J/mol×K	1307.13	Joback Method
dvisc	0.0001450	Pa×s	629.46	Joback Method

dvisc	0.0000772	Pa×s	701.43	Joback Method
dvisc	0.0000462	Pa×s	773.39	Joback Method
dvisc	0.0000302	Pa×s	845.36	Joback Method
dvisc	0.0000211	Pa×s	917.32	Joback Method
dvisc	0.0000155	Pa×s	989.28	Joback Method
dvisc	0.0000119	Pa×s	1061.25	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=U416778&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