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

Inchi: InChI=1S/C26H41ClO5/c1-2-3-4-5-10-15-20-31-25(28)18-11-8-6-7-9-12-19-26(29)32-22-
InchiKey: IMNFXYMBBUECMY-UHFFFAOYSA-N
Formula: C26H41ClO5
SMILES: CCCCCCCCOC(=O)CCCCCCCCC(=O)OCCOc1ccccc1Cl
Mol. weight [g/mol]: 469.05

Physical Properties

Property code	Value	Unit	Source
gf	-313.95	kJ/mol	Joback Method
hf	-992.47	kJ/mol	Joback Method
hfus	67.71	kJ/mol	Joback Method
hvap	101.51	kJ/mol	Joback Method
log10ws	-7.95		Crippen Method
logp	7.287		Crippen Method
mcvol	386.430	ml/mol	McGowan Method
pc	885.77	kPa	Joback Method
rinpol	3152.00		NIST Webbook
rinpol	3152.00		NIST Webbook
tb	1038.37	K	Joback Method
tc	1275.35	K	Joback Method
tf	618.19	K	Joback Method
vc	1.498	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1297.79	J/mol×K	1038.37	Joback Method
cpg	1356.82	J/mol×K	1235.85	Joback Method
cpg	1348.57	J/mol×K	1196.36	Joback Method
cpg	1338.58	J/mol×K	1156.86	Joback Method
cpg	1326.82	J/mol×K	1117.36	Joback Method
cpg	1313.24	J/mol×K	1077.87	Joback Method
cpg	1363.38	J/mol×K	1275.35	Joback Method
dvisc	0.0000140	Pa×s	1038.37	Joback Method

dvisc	0.0000182	Pa×s	968.34	Joback Method
dvisc	0.0000246	Pa×s	898.31	Joback Method
dvisc	0.0000351	Pa×s	828.28	Joback Method
dvisc	0.0000535	Pa×s	758.25	Joback Method
dvisc	0.0000887	Pa×s	688.22	Joback Method
dvisc	0.0001650	Pa×s	618.19	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=U416777&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