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

Inchi: InChI=1S/C26H32Cl2O6/c27-21-11-7-9-13-23(21)31-17-19-33-25(29)15-5-3-1-2-4-6-16-2

InchiKey: KACVKDRQJIHRJF-UHFFFAOYSA-N

Formula: C26H32Cl2O6

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

Mol. weight [g/mol]: 511.44

Physical Properties

Property code	Value	Unit	Source
gf	-328.10	kJ/mol	Joback Method
hf	-915.37	kJ/mol	Joback Method
hfus	66.74	kJ/mol	Joback Method
hvap	111.25	kJ/mol	Joback Method
log10ws	-7.48		Crippen Method
logp	6.658		Crippen Method
mcvol	380.780	ml/mol	McGowan Method
pc	1041.93	kPa	Joback Method
rinpol	3690.00		NIST Webbook
rinpol	3690.00		NIST Webbook
tb	1129.88	K	Joback Method
tc	1384.95	K	Joback Method
tf	709.28	K	Joback Method
vc	1.458	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1225.63	J/mol×K	1129.88	Joback Method
cpg	1234.05	J/mol×K	1172.39	Joback Method
cpg	1240.32	J/mol×K	1214.90	Joback Method
cpg	1244.47	J/mol×K	1257.42	Joback Method
cpg	1246.54	J/mol×K	1299.93	Joback Method
cpg	1246.57	J/mol×K	1342.44	Joback Method
cpg	1244.58	J/mol×K	1384.95	Joback Method
dvisc	0.0000758	Pa×s	709.28	Joback Method

dvisc	0.0000454	Pa×s	779.38	Joback Method
dvisc	0.0000295	Pa×s	849.48	Joback Method
dvisc	0.0000206	Pa×s	919.58	Joback Method
dvisc	0.0000150	Pa×s	989.68	Joback Method
dvisc	0.0000115	Pa×s	1059.78	Joback Method
dvisc	0.0000091	Pa×s	1129.88	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416781&Units=SI
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

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