Sebacic acid, di(2-chlorophenethyl) ester

Inchi: InChI=1S/C26H32Cl2O4/c27-23-13-9-7-11-21(23)17-19-31-25(29)15-5-3-1-2-4-6-16-26(
InchiKey: SJXHUCAISCMPDG-UHFFFAOYSA-N
Formula: C26H32Cl2O4
SMILES: O=C(CCCCCCCCC(=O)OCCc1ccccc1Cl)OCCc1ccccc1Cl
Mol. weight [g/mol]: 479.44

Physical Properties

Property code	Value	Unit	Source
gf	-118.10	kJ/mol	Joback Method
hf	-650.93	kJ/mol	Joback Method
hfus	64.37	kJ/mol	Joback Method
hvap	106.43	kJ/mol	Joback Method
log10ws	-8.01		Crippen Method
logp	6.986		Crippen Method
mcvol	369.040	ml/mol	McGowan Method
pc	1065.18	kPa	Joback Method
rinpol	3355.00		NIST Webbook
rinpol	3355.00		NIST Webbook
tb	1085.04	K	Joback Method
tc	1328.40	K	Joback Method
tf	664.82	K	Joback Method
vc	1.421	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1179.15	J/mol×K	1085.04	Joback Method
cpg	1190.97	J/mol×K	1125.60	Joback Method
cpg	1201.27	J/mol×K	1166.16	Joback Method
cpg	1210.13	J/mol×K	1206.72	Joback Method
cpg	1217.63	J/mol×K	1247.28	Joback Method
cpg	1223.85	J/mol×K	1287.84	Joback Method
cpg	1228.86	J/mol×K	1328.40	Joback Method
dvisc	0.0001559	Pa×s	664.82	Joback Method

dvisc	0.0000904	Pa×s	734.86	Joback Method
dvisc	0.0000576	Pa×s	804.89	Joback Method
dvisc	0.0000395	Pa×s	874.93	Joback Method
dvisc	0.0000286	Pa×s	944.97	Joback Method
dvisc	0.0000217	Pa×s	1015.00	Joback Method
dvisc	0.0000170	Pa×s	1085.04	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=U416235&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