Sebacic acid, di(2-chlorophenyl) ester

Inchi: InChI=1S/C22H24Cl2O4/c23-17-11-7-9-13-19(17)27-21(25)15-5-3-1-2-4-6-16-22(26)28-2
InchiKey: VBUQYFANRSVSSI-UHFFFAOYSA-N
Formula: C22H24Cl2O4
SMILES: O=C(CCCCCCCCC(=O)Oc1ccccc1Cl)Oc1ccccc1Cl
Mol. weight [g/mol]: 423.33

Physical Properties

Property code	Value	Unit	Source
gf	-151.78	kJ/mol	Joback Method
hf	-568.37	kJ/mol	Joback Method
hfus	54.01	kJ/mol	Joback Method
hvap	97.52	kJ/mol	Joback Method
log10ws	-7.63		Crippen Method
logp	6.625		Crippen Method
mcvol	312.680	ml/mol	McGowan Method
pc	1392.29	kPa	Joback Method
rinpol	3302.00		NIST Webbook
rinpol	3302.00		NIST Webbook
tb	993.52	K	Joback Method
tc	1225.45	K	Joback Method
tf	619.74	K	Joback Method
vc	1.198	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	940.76	J/mol×K	993.52	Joback Method
cpg	952.26	J/mol×K	1032.18	Joback Method
cpg	962.43	J/mol×K	1070.83	Joback Method
cpg	971.34	J/mol×K	1109.49	Joback Method
cpg	979.02	J/mol×K	1148.14	Joback Method
cpg	985.52	J/mol×K	1186.80	Joback Method
cpg	990.90	J/mol×K	1225.45	Joback Method
dvisc	0.0002519	Pa×s	619.74	Joback Method

dvisc	0.0001520	Pa×s	682.04	Joback Method
dvisc	0.0000999	Pa×s	744.33	Joback Method
dvisc	0.0000700	Pa×s	806.63	Joback Method
dvisc	0.0000516	Pa×s	868.93	Joback Method
dvisc	0.0000397	Pa×s	931.22	Joback Method
dvisc	0.0000315	Pa×s	993.52	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U354438&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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