Sebacic acid, isohexyl 2,3,5,6-tetrachlorophenyl ester

Inchi: InChI=1S/C22H30Cl4O4/c1-15(2)10-9-13-29-18(27)11-7-5-3-4-6-8-12-19(28)30-22-20(25
InchiKey: WKYLBSZRXPELIO-UHFFFAOYSA-N
Formula: C22H30Cl4O4
SMILES: CC(C)CCCOC(=O)CCCCCCCCC(=O)Oc1c(Cl)c(Cl)cc(Cl)c1Cl
Mol. weight [g/mol]: 500.28

Physical Properties

Property code	Value	Unit	Source
gf	-309.75	kJ/mol	Joback Method
hf	-864.60	kJ/mol	Joback Method
hfus	64.06	kJ/mol	Joback Method
hvap	104.95	kJ/mol	Joback Method
log10ws	-9.01		Crippen Method
logp	8.306		Crippen Method
mcvol	360.920	ml/mol	McGowan Method
pc	1035.90	kPa	Joback Method
rinpol	3319.00		NIST Webbook
rinpol	3319.00		NIST Webbook
tb	1051.22	K	Joback Method
tc	1286.99	K	Joback Method
tf	663.20	K	Joback Method
vc	1.397	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1089.30	J/mol×K	1051.22	Joback Method
cpg	1130.99	J/mol×K	1247.70	Joback Method
cpg	1125.53	J/mol×K	1208.40	Joback Method
cpg	1118.66	J/mol×K	1169.11	Joback Method
cpg	1110.35	J/mol×K	1129.81	Joback Method
cpg	1100.58	J/mol×K	1090.52	Joback Method
cpg	1135.08	J/mol×K	1286.99	Joback Method
dvisc	0.0000203	Pa×s	1051.22	Joback Method

dvisc	0.0000255	Pa×s	986.55	Joback Method
dvisc	0.0000331	Pa×s	921.88	Joback Method
dvisc	0.0000447	Pa×s	857.21	Joback Method
dvisc	0.0000634	Pa×s	792.54	Joback Method
dvisc	0.0000957	Pa×s	727.87	Joback Method
dvisc	0.0001564	Pa×s	663.20	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355293&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