Adipic acid, decyl 2,3,5,6-tetrachlorophenyl ester

Inchi: InChI=1S/C22H30Cl4O4/c1-2-3-4-5-6-7-8-11-14-29-18(27)12-9-10-13-19(28)30-22-20(25
InchiKey: HLHLCIXWRGFATG-UHFFFAOYSA-N
Formula: C22H30Cl4O4
SMILES: CCCCCCCCCCOC(=O)CCCCC(=O)Oc1c(Cl)c(Cl)cc(Cl)c1Cl
Mol. weight [g/mol]: 500.28

Physical Properties

Property code	Value	Unit	Source
gf	-307.31	kJ/mol	Joback Method
hf	-859.32	kJ/mol	Joback Method
hfus	67.58	kJ/mol	Joback Method
hvap	105.34	kJ/mol	Joback Method
log10ws	-9.25		Crippen Method
logp	8.450		Crippen Method
mcvol	360.920	ml/mol	McGowan Method
pc	1030.59	kPa	Joback Method
rinpol	3308.00		NIST Webbook
rinpol	3308.00		NIST Webbook
tb	1051.66	K	Joback Method
tc	1287.64	K	Joback Method
tf	678.20	K	Joback Method
vc	1.403	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1089.01	J/mol×K	1051.66	Joback Method
cpg	1100.39	J/mol×K	1090.99	Joback Method
cpg	1110.27	J/mol×K	1130.32	Joback Method
cpg	1118.70	J/mol×K	1169.65	Joback Method
cpg	1125.71	J/mol×K	1208.98	Joback Method
cpg	1131.32	J/mol×K	1248.31	Joback Method
cpg	1135.56	J/mol×K	1287.64	Joback Method
dvisc	0.0001497	Pa×s	678.20	Joback Method

dvisc	0.0000954	Pa×s	740.44	Joback Method
dvisc	0.0000652	Pa×s	802.69	Joback Method
dvisc	0.0000471	Pa×s	864.93	Joback Method
dvisc	0.0000355	Pa×s	927.17	Joback Method
dvisc	0.0000278	Pa×s	989.42	Joback Method
dvisc	0.0000223	Pa×s	1051.66	Joback Method

Sources

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=U353955&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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