Adipic acid, pentyl 2,3,4,6-tetrachlorophenyl ester

Inchi: InChI=1S/C17H20Cl4O4/c1-2-3-6-9-24-13(22)7-4-5-8-14(23)25-17-12(19)10-11(18)15(20
InchiKey: ZBITWPQNVZHMSW-UHFFFAOYSA-N
Formula: C17H20Cl4O4
SMILES: CCCCCOC(=O)CCCCC(=O)Oc1c(Cl)cc(Cl)c(Cl)c1Cl
Mol. weight [g/mol]: 430.15

Physical Properties

Property code	Value	Unit	Source
gf	-349.41	kJ/mol	Joback Method
hf	-756.12	kJ/mol	Joback Method
hfus	54.63	kJ/mol	Joback Method
hvap	94.21	kJ/mol	Joback Method
log10ws	-7.16		Crippen Method
logp	6.499		Crippen Method
mcvol	290.470	ml/mol	McGowan Method
pc	1440.25	kPa	Joback Method
rinpol	2801.00		NIST Webbook
tb	937.26	K	Joback Method
tc	1157.93	K	Joback Method
tf	621.85	K	Joback Method
vc	1.123	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	796.49	J/mol×K	937.26	Joback Method
cpg	838.14	J/mol×K	1121.15	Joback Method
cpg	832.01	J/mol×K	1084.37	Joback Method
cpg	824.79	J/mol×K	1047.59	Joback Method
cpg	816.47	J/mol×K	1010.82	Joback Method
cpg	807.04	J/mol×K	974.04	Joback Method
cpg	843.19	J/mol×K	1157.93	Joback Method
dvisc	0.0000479	Pa×s	937.26	Joback Method
dvisc	0.0000586	Pa×s	884.69	Joback Method

dvisc	0.0000734	Pa×s	832.12	Joback Method
dvisc	0.0000948	Pa×s	779.56	Joback Method
dvisc	0.0001271	Pa×s	726.99	Joback Method
dvisc	0.0001784	Pa×s	674.42	Joback Method
dvisc	0.0002652	Pa×s	621.85	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=U353915&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