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

Inchi: InChI=1S/C21H28Cl4O4/c1-2-3-10-13-28-17(26)11-8-6-4-5-7-9-12-18(27)29-21-19(24)15
InchiKey: VDCWJTPNVJJVBB-UHFFFAOYSA-N
Formula: C21H28Cl4O4
SMILES: CCCCCOC(=O)CCCCCCCCC(=O)Oc1c(Cl)c(Cl)cc(Cl)c1Cl
Mol. weight [g/mol]: 486.26

Physical Properties

Property code	Value	Unit	Source
gf	-315.73	kJ/mol	Joback Method
hf	-838.68	kJ/mol	Joback Method
hfus	64.99	kJ/mol	Joback Method
hvap	103.12	kJ/mol	Joback Method
log10ws	-8.83		Crippen Method
logp	8.060		Crippen Method
mcvol	346.830	ml/mol	McGowan Method
pc	1097.17	kPa	Joback Method
rinpol	3260.00		NIST Webbook
rinpol	3260.00		NIST Webbook
tb	1028.78	K	Joback Method
tc	1259.68	K	Joback Method
tf	666.93	K	Joback Method
vc	1.347	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1029.49	J/mol×K	1028.78	Joback Method
cpg	1071.95	J/mol×K	1221.20	Joback Method
cpg	1066.14	J/mol×K	1182.71	Joback Method
cpg	1059.02	J/mol×K	1144.23	Joback Method
cpg	1050.56	J/mol×K	1105.75	Joback Method
cpg	1040.72	J/mol×K	1067.26	Joback Method
cpg	1076.46	J/mol×K	1259.68	Joback Method
dvisc	0.0000261	Pa×s	1028.78	Joback Method

dvisc	0.0000323	Pa×s	968.47	Joback Method
dvisc	0.0000412	Pa×s	908.16	Joback Method
dvisc	0.0000544	Pa×s	847.86	Joback Method
dvisc	0.0000749	Pa×s	787.55	Joback Method
dvisc	0.0001087	Pa×s	727.24	Joback Method
dvisc	0.0001687	Pa×s	666.93	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355292&Units=SI

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