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

Inchi: InChI=1S/C23H32Cl4O4/c1-2-3-4-9-12-15-30-19(28)13-10-7-5-6-8-11-14-20(29)31-23-21

InchiKey: VSCJNRRLVWZOOS-UHFFFAOYSA-N

Formula: C23H32Cl4O4

SMILES: CCCCCCCOC(=O)CCCCCCCCC(=O)Oc1c(Cl)c(Cl)cc(Cl)c1Cl

Mol. weight [g/mol]: 514.31

Physical Properties

Property code	Value	Unit	Source
gf	-298.89	kJ/mol	Joback Method
hf	-879.96	kJ/mol	Joback Method
hfus	70.17	kJ/mol	Joback Method
hvap	107.57	kJ/mol	Joback Method
log10ws	-9.67		Crippen Method
logp	8.840		Crippen Method
mcvol	375.010	ml/mol	McGowan Method
pc	969.88	kPa	Joback Method
rinpol	3467.00		NIST Webbook
tb	1074.54	K	Joback Method
tc	1316.76	K	Joback Method
tf	689.47	K	Joback Method
vc	1.460	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1148.94	J/mol×K	1074.54	Joback Method
cpg	1190.95	J/mol×K	1276.39	Joback Method
cpg	1185.59	J/mol×K	1236.02	Joback Method
cpg	1178.74	J/mol×K	1195.65	Joback Method
cpg	1170.37	J/mol×K	1155.28	Joback Method
cpg	1160.45	J/mol×K	1114.91	Joback Method
cpg	1194.88	J/mol×K	1316.76	Joback Method
dvisc	0.0000191	Pa×s	1074.54	Joback Method
dvisc	0.0000238	Pa×s	1010.36	Joback Method

dvisc	0.0000306	Pa×s	946.18	Joback Method
dvisc	0.0000407	Pa×s	882.00	Joback Method
dvisc	0.0000567	Pa×s	817.83	Joback Method
dvisc	0.0000836	Pa×s	753.65	Joback Method
dvisc	0.0001324	Pa×s	689.47	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=U355295&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