Glutaric acid, pentachlorophenyl propyl ester

Inchi: InChI=1S/C14H13Cl5O4/c1-2-6-22-7(20)4-3-5-8(21)23-14-12(18)10(16)9(15)11(17)13(14
InchiKey: NEHBKZXPCPEVLA-UHFFFAOYSA-N
Formula: C14H13Cl5O4
SMILES: CCCOC(=O)CCCC(=O)Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl
Mol. weight [g/mol]: 422.52

Physical Properties

Property code	Value	Unit	Source
gf	-396.23	kJ/mol	Joback Method
hf	-721.41	kJ/mol	Joback Method
hfus	50.67	kJ/mol	Joback Method
hvap	92.58	kJ/mol	Joback Method
log10ws	-6.58		Crippen Method
logp	5.982		Crippen Method
mcvol	260.440	ml/mol	McGowan Method
pc	1737.56	kPa	Joback Method
rinpol	2691.00		NIST Webbook
tb	911.03	K	Joback Method
tc	1137.46	K	Joback Method
tf	630.48	K	Joback Method
vc	1.004	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	645.69	J/mol×K	911.03	Joback Method
cpg	654.25	J/mol×K	948.77	Joback Method
cpg	661.81	J/mol×K	986.51	Joback Method
cpg	668.36	J/mol×K	1024.25	Joback Method
cpg	673.89	J/mol×K	1061.99	Joback Method
cpg	678.40	J/mol×K	1099.73	Joback Method
cpg	681.87	J/mol×K	1137.46	Joback Method
dvisc	0.0002793	Pa×s	630.48	Joback Method
dvisc	0.0002011	Pa×s	677.24	Joback Method

dvisc	0.0001511	Pa×s	724.00	Joback Method
dvisc	0.0001175	Pa×s	770.75	Joback Method
dvisc	0.0000941	Pa×s	817.51	Joback Method
dvisc	0.0000771	Pa×s	864.27	Joback Method
dvisc	0.0000646	Pa×s	911.03	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=U360252&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