Glutaric acid, ethyl pentachlorophenyl ester

Inchi: InChI=1S/C13H11Cl5O4/c1-2-21-6(19)4-3-5-7(20)22-13-11(17)9(15)8(14)10(16)12(13)18
InchiKey: BTUGUQUIQVXBBT-UHFFFAOYSA-N
Formula: C13H11Cl5O4
SMILES: CCOC(=O)CCCC(=O)Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl
Mol. weight [g/mol]: 408.49

Physical Properties

Property code	Value	Unit	Source
gf	-404.65	kJ/mol	Joback Method
hf	-700.77	kJ/mol	Joback Method
hfus	48.08	kJ/mol	Joback Method
hvap	90.36	kJ/mol	Joback Method
log10ws	-6.17		Crippen Method
logp	5.592		Crippen Method
mcvol	246.350	ml/mol	McGowan Method
pc	1885.44	kPa	Joback Method
rinpol	2589.00		NIST Webbook
rinpol	2589.00		NIST Webbook
tb	888.15	K	Joback Method
tc	1116.03	K	Joback Method
tf	619.21	K	Joback Method
vc	0.949	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	591.13	J/mol×K	888.15	Joback Method
cpg	622.74	J/mol×K	1078.05	Joback Method
cpg	618.36	J/mol×K	1040.07	Joback Method
cpg	613.00	J/mol×K	1002.09	Joback Method
cpg	606.66	J/mol×K	964.11	Joback Method
cpg	599.37	J/mol×K	926.13	Joback Method
cpg	626.12	J/mol×K	1116.03	Joback Method
dvisc	0.0000746	Pa×s	888.15	Joback Method

dvisc	0.0000887	Pa×s	843.33	Joback Method
dvisc	0.0001076	Pa×s	798.50	Joback Method
dvisc	0.0001336	Pa×s	753.68	Joback Method
dvisc	0.0001705	Pa×s	708.86	Joback Method
dvisc	0.0002249	Pa×s	664.03	Joback Method
dvisc	0.0003086	Pa×s	619.21	Joback Method

Sources

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=U360251&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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