Glutaric acid, hexyl pentachlorophenyl ester

Inchi: InChI=1S/C17H19Cl5O4/c1-2-3-4-5-9-25-10(23)7-6-8-11(24)26-17-15(21)13(19)12(18)14
InchiKey: LJWJFVLDUHIUJV-UHFFFAOYSA-N
Formula: C17H19Cl5O4
SMILES: CCCCCCOC(=O)CCCC(=O)Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl
Mol. weight [g/mol]: 464.60

Physical Properties

Property code	Value	Unit	Source
gf	-370.97	kJ/mol	Joback Method
hf	-783.33	kJ/mol	Joback Method
hfus	58.44	kJ/mol	Joback Method
hvap	99.26	kJ/mol	Joback Method
log10ws	-7.84		Crippen Method
logp	7.153		Crippen Method
mcvol	302.710	ml/mol	McGowan Method
pc	1385.05	kPa	Joback Method
rinpol	3018.00		NIST Webbook
tb	979.67	K	Joback Method
tc	1206.48	K	Joback Method
tf	664.29	K	Joback Method
vc	1.173	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	813.93	J/mol×K	979.67	Joback Method
cpg	823.16	J/mol×K	1017.47	Joback Method
cpg	831.22	J/mol×K	1055.27	Joback Method
cpg	838.11	J/mol×K	1093.08	Joback Method
cpg	843.83	J/mol×K	1130.88	Joback Method
cpg	848.38	J/mol×K	1168.68	Joback Method
cpg	851.78	J/mol×K	1206.48	Joback Method
dvisc	0.0002031	Pa×s	664.29	Joback Method
dvisc	0.0001414	Pa×s	716.85	Joback Method

dvisc	0.0001034	Pa×s	769.42	Joback Method
dvisc	0.0000787	Pa×s	821.98	Joback Method
dvisc	0.0000619	Pa×s	874.54	Joback Method
dvisc	0.0000501	Pa×s	927.11	Joback Method
dvisc	0.0000414	Pa×s	979.67	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=U360256&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