Glutaric acid, heptyl pentachlorophenyl ester

Inchi: InChI=1S/C18H21Cl5O4/c1-2-3-4-5-6-10-26-11(24)8-7-9-12(25)27-18-16(22)14(20)13(19
InchiKey: OEKJGOADKAMYDC-UHFFFAOYSA-N
Formula: C18H21Cl5O4
SMILES: CCCCCCCOC(=O)CCCC(=O)Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl
Mol. weight [g/mol]: 478.62

Physical Properties

Property code	Value	Unit	Source
gf	-362.55	kJ/mol	Joback Method
hf	-803.97	kJ/mol	Joback Method
hfus	61.03	kJ/mol	Joback Method
hvap	101.48	kJ/mol	Joback Method
log10ws	-8.26		Crippen Method
logp	7.543		Crippen Method
mcvol	316.800	ml/mol	McGowan Method
pc	1291.14	kPa	Joback Method
rinpol	3121.00		NIST Webbook
rinpol	3121.00		NIST Webbook
tb	1002.55	K	Joback Method
tc	1231.23	K	Joback Method
tf	675.56	K	Joback Method
vc	1.228	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	871.30	J/mol×K	1002.55	Joback Method
cpg	880.69	J/mol×K	1040.66	Joback Method
cpg	888.85	J/mol×K	1078.78	Joback Method
cpg	895.76	J/mol×K	1116.89	Joback Method
cpg	901.45	J/mol×K	1155.00	Joback Method
cpg	905.92	J/mol×K	1193.12	Joback Method
cpg	909.17	J/mol×K	1231.23	Joback Method
dvisc	0.0001815	Pa×s	675.56	Joback Method

dvisc	0.0001250	Pa×s	730.06	Joback Method
dvisc	0.0000906	Pa×s	784.56	Joback Method
dvisc	0.0000685	Pa×s	839.05	Joback Method
dvisc	0.0000536	Pa×s	893.55	Joback Method
dvisc	0.0000432	Pa×s	948.05	Joback Method
dvisc	0.0000356	Pa×s	1002.55	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=U360257&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