Glutaric acid, decyl pentachlorophenyl ester

Inchi: InChI=1S/C21H27Cl5O4/c1-2-3-4-5-6-7-8-9-13-29-14(27)11-10-12-15(28)30-21-19(25)17
InchiKey: VRPVTFWUACZCSF-UHFFFAOYSA-N
Formula: C21H27Cl5O4
SMILES: CCCCCCCCCCOC(=O)CCCC(=O)Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl
Mol. weight [g/mol]: 520.70

Physical Properties

Property code	Value	Unit	Source
gf	-337.29	kJ/mol	Joback Method
hf	-865.89	kJ/mol	Joback Method
hfus	68.80	kJ/mol	Joback Method
hvap	108.16	kJ/mol	Joback Method
log10ws	-9.51		Crippen Method
logp	8.713		Crippen Method
mcvol	359.070	ml/mol	McGowan Method
pc	1060.33	kPa	Joback Method
rinpol	3434.00		NIST Webbook
rinpol	3434.00		NIST Webbook
tb	1071.19	K	Joback Method
tc	1311.50	K	Joback Method
tf	709.37	K	Joback Method
vc	1.397	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1046.50	J/mol×K	1071.19	Joback Method
cpg	1056.25	J/mol×K	1111.24	Joback Method
cpg	1064.50	J/mol×K	1151.29	Joback Method
cpg	1071.28	J/mol×K	1191.35	Joback Method
cpg	1076.60	J/mol×K	1231.40	Joback Method
cpg	1080.48	J/mol×K	1271.45	Joback Method
cpg	1082.96	J/mol×K	1311.50	Joback Method
dvisc	0.0001275	Pa×s	709.37	Joback Method

dvisc	0.0000852	Pa×s	769.67	Joback Method
dvisc	0.0000603	Pa×s	829.98	Joback Method
dvisc	0.0000447	Pa×s	890.28	Joback Method
dvisc	0.0000345	Pa×s	950.58	Joback Method
dvisc	0.0000274	Pa×s	1010.89	Joback Method
dvisc	0.0000223	Pa×s	1071.19	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=U360260&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