Glutaric acid, 2,4,6-trichlorophenyl trans-4-tert-butylcyclohexyl ester

Inchi: InChI=1S/C21H27Cl3O4/c1-21(2,3)13-7-9-15(10-8-13)27-18(25)5-4-6-19(26)28-20-16(23
InchiKey: RZNLJEODKODEMK-UHFFFAOYSA-N
Formula: C21H27Cl3O4
SMILES: CC(C)(C)C1CCC(OC(=O)CCCC(=O)Oc2c(Cl)cc(Cl)cc2Cl)CC1
Mol. weight [g/mol]: 449.80

Physical Properties

Property code	Value	Unit	Source
gf	-274.59	kJ/mol	Joback Method
hf	-786.24	kJ/mol	Joback Method
hfus	46.68	kJ/mol	Joback Method
hvap	96.89	kJ/mol	Joback Method
log10ws	-7.67		Crippen Method
logp	6.871		Crippen Method
mcvol	323.730	ml/mol	McGowan Method
pc	1297.66	kPa	Joback Method
rinpol	3087.00		NIST Webbook
rinpol	3087.00		NIST Webbook
tb	998.02	K	Joback Method
tc	1236.30	K	Joback Method
tf	630.05	K	Joback Method
vc	1.220	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1007.48	J/mol×K	998.02	Joback Method
cpg	1019.92	J/mol×K	1037.73	Joback Method
cpg	1030.75	J/mol×K	1077.45	Joback Method
cpg	1040.05	J/mol×K	1117.16	Joback Method
cpg	1047.86	J/mol×K	1156.88	Joback Method
cpg	1054.23	J/mol×K	1196.59	Joback Method
cpg	1059.22	J/mol×K	1236.30	Joback Method
dvisc	0.0002512	Pa×s	630.05	Joback Method

dvisc	0.0001527	Pa×s	691.38	Joback Method
dvisc	0.0001007	Pa×s	752.71	Joback Method
dvisc	0.0000707	Pa×s	814.04	Joback Method
dvisc	0.0000521	Pa×s	875.36	Joback Method
dvisc	0.0000400	Pa×s	936.69	Joback Method
dvisc	0.0000317	Pa×s	998.02	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393409&Units=SI
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

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