Glutaric acid, 3-chlorophenyl trans-4-tert-butylcyclohexyl ester

Inchi: InChI=1S/C21H29ClO4/c1-21(2,3)15-10-12-17(13-11-15)25-19(23)8-5-9-20(24)26-18-7-4

InchiKey: QEEYFQADBLTCOI-UHFFFAOYSA-N

Formula: C21H29ClO4

SMILES: CC(C)(C)C1CCC(OC(=O)CCCC(=O)Oc2cccc(Cl)c2)CC1

Mol. weight [g/mol]: 380.91

Physical Properties

Property code	Value	Unit	Source
gf	-231.47	kJ/mol	Joback Method
hf	-731.82	kJ/mol	Joback Method
hfus	39.06	kJ/mol	Joback Method
hvap	86.80	kJ/mol	Joback Method
log10ws	-6.30		Crippen Method
logp	5.564		Crippen Method
mcvol	299.250	ml/mol	McGowan Method
pc	1400.64	kPa	Joback Method
rinpol	2814.00		NIST Webbook
rinpol	2814.00		NIST Webbook
tb	913.20	K	Joback Method
tc	1141.97	K	Joback Method
tf	545.17	K	Joback Method
vc	1.121	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	963.65	J/mol×K	913.20	Joback Method
cpg	1028.17	J/mol×K	1103.84	Joback Method
cpg	1018.21	J/mol×K	1065.71	Joback Method
cpg	1006.83	J/mol×K	1027.58	Joback Method
cpg	993.98	J/mol×K	989.46	Joback Method
cpg	979.61	J/mol×K	951.33	Joback Method
cpg	1036.79	J/mol×K	1141.97	Joback Method
dvisc	0.0000428	Pa×s	913.20	Joback Method

dvisc	0.0000555	Pa×s	851.86	Joback Method
dvisc	0.0000750	Pa×s	790.52	Joback Method
dvisc	0.0001065	Pa×s	729.18	Joback Method
dvisc	0.0001612	Pa×s	667.85	Joback Method
dvisc	0.0002655	Pa×s	606.51	Joback Method
dvisc	0.0004893	Pa×s	545.17	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393406&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