Glutaric acid, 2-chloro-6-fluorophenyl trans-4-tert-butylcyclohexyl ester

Inchi: InChI=1S/C21H28ClFO4/c1-21(2,3)14-10-12-15(13-11-14)26-18(24)8-5-9-19(25)27-20-1

InchiKey: NVGCGTPYSWKYPJ-UHFFFAOYSA-N

Formula: C21H28ClFO4

SMILES: CC(C)(C)C1CCC(OC(=O)CCCC(=O)Oc2c(F)cccc2Cl)CC1

Mol. weight [g/mol]: 398.90

Physical Properties

Property code	Value	Unit	Source
gf	-435.91	kJ/mol	Joback Method
hf	-939.40	kJ/mol	Joback Method
hfus	41.75	kJ/mol	Joback Method
hvap	86.64	kJ/mol	Joback Method
log10ws	-6.63		Crippen Method
logp	5.703		Crippen Method
mcvol	301.020	ml/mol	McGowan Method
pc	1339.80	kPa	Joback Method
rinpol	2765.00		NIST Webbook
rinpol	2765.00		NIST Webbook
tb	917.45	K	Joback Method
tc	1141.28	K	Joback Method
tf	558.28	K	Joback Method
vc	1.139	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	969.86	J/mol×K	917.45	Joback Method
cpg	985.17	J/mol×K	954.75	Joback Method
cpg	998.97	J/mol×K	992.06	Joback Method
cpg	1011.29	J/mol×K	1029.36	Joback Method
cpg	1022.18	J/mol×K	1066.67	Joback Method
cpg	1031.69	J/mol×K	1103.97	Joback Method
cpg	1039.87	J/mol×K	1141.28	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=U393405&Units=SI

Legend

cpg:	Ideal gas heat capacity
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