Glutaric acid, 2-chloro-6-fluorophenyl 3,7-dimethyloctyl ester

Inchi: InChI=1S/C21H30ClFO4/c1-15(2)7-4-8-16(3)13-14-26-19(24)11-6-12-20(25)27-21-17(22
InchiKey: OZDKFIGZJQDXBW-UHFFFAOYSA-N
Formula: C21H30ClFO4
SMILES: CC(C)CCCC(C)CCOC(=O)CCCC(=O)Oc1c(F)cccc1Cl
Mol. weight [g/mol]: 400.91

Physical Properties

Property code	Value	Unit	Source
gf	-460.37	kJ/mol	Joback Method
hf	-975.19	kJ/mol	Joback Method
hfus	49.21	kJ/mol	Joback Method
hvap	87.04	kJ/mol	Joback Method
log10ws	-6.62		Crippen Method
logp	5.950		Crippen Method
mcvol	311.880	ml/mol	McGowan Method
pc	1183.34	kPa	Joback Method
rinpol	2600.00		NIST Webbook
rinpol	2600.00		NIST Webbook
tb	904.92	K	Joback Method
tc	1112.38	K	Joback Method
tf	522.72	K	Joback Method
vc	1.206	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	971.63	J/mol×K	904.92	Joback Method
cpg	986.51	J/mol×K	939.50	Joback Method
cpg	1000.15	J/mol×K	974.07	Joback Method
cpg	1012.59	J/mol×K	1008.65	Joback Method
cpg	1023.83	J/mol×K	1043.23	Joback Method
cpg	1033.92	J/mol×K	1077.80	Joback Method
cpg	1042.87	J/mol×K	1112.38	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391487&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
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