Glutaric acid, 2-chloro-6-fluorophenyl 2,4,4-trimethylpentyl ester

Inchi: InChI=1S/C19H26ClFO4/c1-13(11-19(2,3)4)12-24-16(22)9-6-10-17(23)25-18-14(20)7-5-8

InchiKey: QZVCTGWZWWHZMM-UHFFFAOYSA-N

Formula: C19H26ClFO4

SMILES: CC(COC(=O)CCCC(=O)Oc1c(F)cccc1Cl)CC(C)(C)C

Mol. weight [g/mol]: 372.86

Physical Properties

Property code	Value	Unit	Source
gf	-471.93	kJ/mol	Joback Method
hf	-937.38	kJ/mol	Joback Method
hfus	40.14	kJ/mol	Joback Method
hvap	81.68	kJ/mol	Joback Method
log10ws	-5.79		Crippen Method
logp	5.170		Crippen Method
mcvol	283.700	ml/mol	McGowan Method
pc	1367.69	kPa	Joback Method
rinpol	2339.00		NIST Webbook
rinpol	2339.00		NIST Webbook
tb	856.37	K	Joback Method
tc	1064.14	K	Joback Method
tf	517.60	K	Joback Method
vc	1.089	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	854.29	J/mol×K	856.37	Joback Method
cpg	868.78	J/mol×K	891.00	Joback Method
cpg	882.16	J/mol×K	925.63	Joback Method
cpg	894.47	J/mol×K	960.26	Joback Method
cpg	905.75	J/mol×K	994.89	Joback Method
cpg	916.04	J/mol×K	1029.51	Joback Method
cpg	925.37	J/mol×K	1064.14	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391535&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