Glutaric acid, 2-chloro-6-fluorophenyl 2-isopropylphenyl ester

Inchi: InChI=1S/C20H20ClFO4/c1-13(2)14-7-3-4-10-17(14)25-18(23)11-6-12-19(24)26-20-15(2

InchiKey: AFUSJXBXBBISFU-UHFFFAOYSA-N

Formula: C20H20ClFO4

SMILES: CC(C)c1ccccc1OC(=O)CCCC(=O)Oc1c(F)cccc1Cl

Mol. weight [g/mol]: 378.82

Physical Properties

Property code	Value	Unit	Source
gf	-363.57	kJ/mol	Joback Method
hf	-724.21	kJ/mol	Joback Method
hfus	43.80	kJ/mol	Joback Method
hvap	88.14	kJ/mol	Joback Method
log10ws	-6.37		Crippen Method
logp	5.284		Crippen Method
mcvol	274.030	ml/mol	McGowan Method
pc	1596.17	kPa	Joback Method
rinpol	2606.00		NIST Webbook
rinpol	2606.00		NIST Webbook
tb	914.14	K	Joback Method
tc	1139.63	K	Joback Method
tf	565.39	K	Joback Method
vc	1.048	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	809.77	J/mol×K	914.14	Joback Method
cpg	822.02	J/mol×K	951.72	Joback Method
cpg	833.00	J/mol×K	989.30	Joback Method
cpg	842.73	J/mol×K	1026.88	Joback Method
cpg	851.25	J/mol×K	1064.46	Joback Method
cpg	858.58	J/mol×K	1102.04	Joback Method
cpg	864.75	J/mol×K	1139.63	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391922&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

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