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

Inchi: InChI=1S/C14H16ClFO4/c1-9(2)19-12(17)7-4-8-13(18)20-14-10(15)5-3-6-11(14)16/h3,5-

InchiKey: ODXBTPXPFAMCRM-UHFFFAOYSA-N

Formula: C14H16ClFO4

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

Mol. weight [g/mol]: 302.73

Physical Properties

Property code	Value	Unit	Source
gf	-516.87	kJ/mol	Joback Method
hf	-825.43	kJ/mol	Joback Method
hfus	34.61	kJ/mol	Joback Method
hvap	71.85	kJ/mol	Joback Method
log10ws	-4.29		Crippen Method
logp	3.506		Crippen Method
mcvol	213.250	ml/mol	McGowan Method
pc	1987.66	kPa	Joback Method
rinpol	1890.00		NIST Webbook
rinpol	1890.00		NIST Webbook
tb	745.20	K	Joback Method
tc	951.12	K	Joback Method
tf	458.83	K	Joback Method
vc	0.821	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	573.21	J/mol×K	745.20	Joback Method
cpg	586.08	J/mol×K	779.52	Joback Method
cpg	598.07	J/mol×K	813.84	Joback Method
cpg	609.18	J/mol×K	848.16	Joback Method
cpg	619.42	J/mol×K	882.48	Joback Method
cpg	628.79	J/mol×K	916.80	Joback Method
cpg	637.29	J/mol×K	951.12	Joback Method

Sources

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=U393378&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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