Glutaric acid, 2-fluorophenyl isopropyl ester

Inchi: InChI=1S/C14H17FO4/c1-10(2)18-13(16)8-5-9-14(17)19-12-7-4-3-6-11(12)15/h3-4,6-7,1
InchiKey: XPGGZVFBXMRMFH-UHFFFAOYSA-N
Formula: C14H17FO4
SMILES: CC(C)OC(=O)CCCC(=O)Oc1ccccc1F
Mol. weight [g/mol]: 268.28

Physical Properties

Property code	Value	Unit	Source
gf	-495.31	kJ/mol	Joback Method
hf	-798.22	kJ/mol	Joback Method
hfus	30.80	kJ/mol	Joback Method
hvap	66.80	kJ/mol	Joback Method
log10ws	-3.60		Crippen Method
logp	2.853		Crippen Method
mcvol	201.010	ml/mol	McGowan Method
pc	2083.12	kPa	Joback Method
rinpol	1762.00		NIST Webbook
rinpol	1762.00		NIST Webbook
tb	702.79	K	Joback Method
tc	904.30	K	Joback Method
tf	416.39	K	Joback Method
vc	0.771	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	548.41	J/mol×K	702.79	Joback Method
cpg	562.43	J/mol×K	736.37	Joback Method
cpg	575.58	J/mol×K	769.96	Joback Method
cpg	587.86	J/mol×K	803.54	Joback Method
cpg	599.28	J/mol×K	837.13	Joback Method
cpg	609.84	J/mol×K	870.71	Joback Method
cpg	619.56	J/mol×K	904.30	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=U393375&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