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

Inchi: InChI=1S/C19H27FO4/c1-14(12-19(2,3)4)13-23-17(21)10-7-11-18(22)24-16-9-6-5-8-15(1

InchiKey: LHGYJCLZQLHEEJ-UHFFFAOYSA-N

Formula: C19H27FO4

SMILES: CC(COC(=O)CCCC(=O)Oc1ccccc1F)CC(C)(C)C

Mol. weight [g/mol]: 338.41

Physical Properties

Property code	Value	Unit	Source
gf	-450.37	kJ/mol	Joback Method
hf	-910.17	kJ/mol	Joback Method
hfus	36.33	kJ/mol	Joback Method
hvap	76.64	kJ/mol	Joback Method
log10ws	-5.10		Crippen Method
logp	4.517		Crippen Method
mcvol	271.460	ml/mol	McGowan Method
pc	1421.85	kPa	Joback Method
rinpol	2193.00		NIST Webbook
rinpol	2193.00		NIST Webbook
tb	813.96	K	Joback Method
tc	1016.40	K	Joback Method
tf	475.16	K	Joback Method
vc	1.040	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	828.36	J/mol×K	813.96	Joback Method
cpg	844.14	J/mol×K	847.70	Joback Method
cpg	858.80	J/mol×K	881.44	Joback Method
cpg	872.40	J/mol×K	915.18	Joback Method
cpg	884.96	J/mol×K	948.92	Joback Method
cpg	896.53	J/mol×K	982.66	Joback Method
cpg	907.15	J/mol×K	1016.40	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=U391532&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