Glutaric acid, 2-fluorophenyl 2,3-dimethylphenyl ester

Inchi: InChI=1S/C19H19FO4/c1-13-7-5-10-16(14(13)2)23-18(21)11-6-12-19(22)24-17-9-4-3-8-1

InchiKey: DOAPFHPEXFVRQE-UHFFFAOYSA-N

Formula: C19H19FO4

SMILES: Cc1cccc(OC(=O)CCCC(=O)Oc2ccccc2F)c1C

Mol. weight [g/mol]: 330.35

Physical Properties

Property code	Value	Unit	Source
gf	-357.62	kJ/mol	Joback Method
hf	-682.55	kJ/mol	Joback Method
hfus	40.53	kJ/mol	Joback Method
hvap	81.92	kJ/mol	Joback Method
log10ws	-5.45		Crippen Method
logp	4.124		Crippen Method
mcvol	247.700	ml/mol	McGowan Method
pc	1768.38	kPa	Joback Method
rinpol	2510.00		NIST Webbook
rinpol	2510.00		NIST Webbook
tb	854.27	K	Joback Method
tc	1074.69	K	Joback Method
tf	539.20	K	Joback Method
vc	0.950	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	729.45	J/mol×K	854.27	Joback Method
cpg	742.81	J/mol×K	891.01	Joback Method
cpg	754.98	J/mol×K	927.74	Joback Method
cpg	765.97	J/mol×K	964.48	Joback Method
cpg	775.80	J/mol×K	1001.21	Joback Method
cpg	784.50	J/mol×K	1037.95	Joback Method
cpg	792.08	J/mol×K	1074.69	Joback Method

Sources

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=U392221&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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