Glutaric acid, 2-fluorophenyl 3-methylphenyl ester

Inchi: InChI=1S/C18H17FO4/c1-13-6-4-7-14(12-13)22-17(20)10-5-11-18(21)23-16-9-3-2-8-15(1

InchiKey: GXERONDDVMGCCZ-UHFFFAOYSA-N

Formula: C18H17FO4

SMILES: Cc1cccc(OC(=O)CCCC(=O)Oc2ccccc2F)c1

Mol. weight [g/mol]: 316.32

Physical Properties

Property code	Value	Unit	Source
gf	-356.41	kJ/mol	Joback Method
hf	-650.44	kJ/mol	Joback Method
hfus	38.33	kJ/mol	Joback Method
hvap	79.03	kJ/mol	Joback Method
log10ws	-4.97		Crippen Method
logp	3.815		Crippen Method
mcvol	233.610	ml/mol	McGowan Method
pc	1945.79	kPa	Joback Method
rinpol	2389.00		NIST Webbook
rinpol	2389.00		NIST Webbook
tb	826.41	K	Joback Method
tc	1048.06	K	Joback Method
tf	515.41	K	Joback Method
vc	0.893	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	674.47	J/mol×K	826.41	Joback Method
cpg	687.76	J/mol×K	863.35	Joback Method
cpg	699.87	J/mol×K	900.29	Joback Method
cpg	710.85	J/mol×K	937.23	Joback Method
cpg	720.70	J/mol×K	974.18	Joback Method
cpg	729.47	J/mol×K	1011.12	Joback Method
cpg	737.16	J/mol×K	1048.06	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=U391956&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