Glutaric acid, 2-fluorophenyl 2-methoxyphenyl ester

Inchi: InChI=1S/C18H17FO5/c1-22-15-9-4-5-10-16(15)24-18(21)12-6-11-17(20)23-14-8-3-2-7-1

InchiKey: FISGLTSUDQLLSS-UHFFFAOYSA-N

Formula: C18H17FO5

SMILES: COc1ccccc1OC(=O)CCCC(=O)Oc1ccccc1F

Mol. weight [g/mol]: 332.32

Physical Properties

Property code	Value	Unit	Source
gf	-461.41	kJ/mol	Joback Method
hf	-782.66	kJ/mol	Joback Method
hfus	39.52	kJ/mol	Joback Method
hvap	81.44	kJ/mol	Joback Method
log10ws	-4.62		Crippen Method
logp	3.516		Crippen Method
mcvol	239.480	ml/mol	McGowan Method
pc	1916.94	kPa	Joback Method
rinpol	2502.00		NIST Webbook
rinpol	2502.00		NIST Webbook
tb	848.83	K	Joback Method
tc	1069.21	K	Joback Method
tf	537.64	K	Joback Method
vc	0.911	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	700.99	J/mol×K	848.83	Joback Method
cpg	713.70	J/mol×K	885.56	Joback Method
cpg	725.18	J/mol×K	922.29	Joback Method
cpg	735.44	J/mol×K	959.02	Joback Method
cpg	744.48	J/mol×K	995.75	Joback Method
cpg	752.30	J/mol×K	1032.48	Joback Method
cpg	758.93	J/mol×K	1069.21	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391760&Units=SI
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

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