Glutaric acid, 2-fluorophenyl 2,6-dimethoxyphenyl ester

Inchi: InChI=1S/C19H19FO6/c1-23-15-9-5-10-16(24-2)19(15)26-18(22)12-6-11-17(21)25-14-8-

InchiKey: YXSZYMBBMVGLGW-UHFFFAOYSA-N

Formula: C19H19FO6

SMILES: COc1cccc(OC)c1OC(=O)CCCC(=O)Oc1ccccc1F

Mol. weight [g/mol]: 362.35

Physical Properties

Property code	Value	Unit	Source
gf	-567.62	kJ/mol	Joback Method
hf	-946.99	kJ/mol	Joback Method
hfus	42.91	kJ/mol	Joback Method
hvap	86.74	kJ/mol	Joback Method
log10ws	-4.74		Crippen Method
logp	3.524		Crippen Method
mcvol	259.440	ml/mol	McGowan Method
pc	1718.88	kPa	Joback Method
rinpol	2693.00		NIST Webbook
rinpol	2693.00		NIST Webbook
tb	899.11	K	Joback Method
tc	1118.69	K	Joback Method
tf	583.66	K	Joback Method
vc	0.986	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	782.76	J/mol×K	899.11	Joback Method
cpg	794.77	J/mol×K	935.71	Joback Method
cpg	805.39	J/mol×K	972.30	Joback Method
cpg	814.60	J/mol×K	1008.90	Joback Method
cpg	822.40	J/mol×K	1045.49	Joback Method
cpg	828.78	J/mol×K	1082.09	Joback Method
cpg	833.71	J/mol×K	1118.69	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392005&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