Glutaric acid, 2-fluorophenyl 4-methoxybenzyl ester

Inchi: InChI=1S/C19H19FO5/c1-23-15-11-9-14(10-12-15)13-24-18(21)7-4-8-19(22)25-17-6-3-2

InchiKey: XAWRJWWUZLKFLA-UHFFFAOYSA-N

Formula: C19H19FO5

SMILES: COc1ccc(COC(=O)CCCC(=O)Oc2ccccc2F)cc1

Mol. weight [g/mol]: 346.35

Physical Properties

Property code	Value	Unit	Source
gf	-452.99	kJ/mol	Joback Method
hf	-803.30	kJ/mol	Joback Method
hfus	42.11	kJ/mol	Joback Method
hvap	83.67	kJ/mol	Joback Method
log10ws	-4.88		Crippen Method
logp	3.653		Crippen Method
mcvol	253.570	ml/mol	McGowan Method
pc	1765.41	kPa	Joback Method
rinpol	2680.00		NIST Webbook
rinpol	2680.00		NIST Webbook
tb	871.71	K	Joback Method
tc	1090.66	K	Joback Method
tf	548.91	K	Joback Method
vc	0.968	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	757.50	J/mol×K	871.71	Joback Method
cpg	770.34	J/mol×K	908.20	Joback Method
cpg	781.90	J/mol×K	944.69	Joback Method
cpg	792.21	J/mol×K	981.18	Joback Method
cpg	801.27	J/mol×K	1017.68	Joback Method
cpg	809.09	J/mol×K	1054.17	Joback Method
cpg	815.68	J/mol×K	1090.66	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=U391742&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