Glutaric acid, 2-fluorophenyl 3-phenylpropyl ester

Inchi: InChI=1S/C20H21FO4/c21-17-11-4-5-12-18(17)25-20(23)14-6-13-19(22)24-15-7-10-16-8

InchiKey: IKEYUFXQILWJQE-UHFFFAOYSA-N

Formula: C20H21FO4

SMILES: O=C(CCCC(=O)Oc1ccccc1F)OCCCc1ccccc1

Mol. weight [g/mol]: 344.38

Physical Properties

Property code	Value	Unit	Source
gf	-329.94	kJ/mol	Joback Method
hf	-680.25	kJ/mol	Joback Method
hfus	43.90	kJ/mol	Joback Method
hvap	82.82	kJ/mol	Joback Method
log10ws	-5.11		Crippen Method
logp	4.077		Crippen Method
mcvol	261.790	ml/mol	McGowan Method
pc	1674.16	kPa	Joback Method
rinpol	2616.00		NIST Webbook
rinpol	2616.00		NIST Webbook
tb	867.19	K	Joback Method
tc	1084.72	K	Joback Method
tf	525.43	K	Joback Method
vc	1.006	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	788.82	J/mol×K	867.19	Joback Method
cpg	802.52	J/mol×K	903.44	Joback Method
cpg	815.00	J/mol×K	939.70	Joback Method
cpg	826.30	J/mol×K	975.95	Joback Method
cpg	836.46	J/mol×K	1012.21	Joback Method
cpg	845.52	J/mol×K	1048.46	Joback Method
cpg	853.52	J/mol×K	1084.72	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=U391775&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