Glutaric acid, 2-fluorophenyl 2-isopropoxyphenyl ester

Inchi: InChI=1S/C20H21FO5/c1-14(2)24-17-10-5-6-11-18(17)26-20(23)13-7-12-19(22)25-16-9-

InchiKey: FTWKSCWAQUIBAV-UHFFFAOYSA-N

Formula: C20H21FO5

SMILES: CC(C)Oc1ccccc1OC(=O)CCCC(=O)Oc1ccccc1F

Mol. weight [g/mol]: 360.38

Physical Properties

Property code	Value	Unit	Source
gf	-447.01	kJ/mol	Joback Method
hf	-829.22	kJ/mol	Joback Method
hfus	41.18	kJ/mol	Joback Method
hvap	85.51	kJ/mol	Joback Method
log10ws	-5.57		Crippen Method
logp	4.294		Crippen Method
mcvol	267.660	ml/mol	McGowan Method
pc	1641.76	kPa	Joback Method
rinpol	2552.00		NIST Webbook
rinpol	2552.00		NIST Webbook
tb	894.15	K	Joback Method
tc	1114.64	K	Joback Method
tf	545.18	K	Joback Method
vc	1.018	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	815.29	J/mol×K	894.15	Joback Method
cpg	828.32	J/mol×K	930.90	Joback Method
cpg	839.99	J/mol×K	967.65	Joback Method
cpg	850.33	J/mol×K	1004.39	Joback Method
cpg	859.35	J/mol×K	1041.14	Joback Method
cpg	867.06	J/mol×K	1077.89	Joback Method
cpg	873.47	J/mol×K	1114.64	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=U391873&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