Glutaric acid, 2-fluorophenyl 4-methylpent-2-yl ester

Inchi: InChI=1S/C17H23FO4/c1-12(2)11-13(3)21-16(19)9-6-10-17(20)22-15-8-5-4-7-14(15)18/h

InchiKey: IYSAPCYDTDPTEU-UHFFFAOYSA-N

Formula: C17H23FO4

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

Mol. weight [g/mol]: 310.36

Physical Properties

Property code	Value	Unit	Source
gf	-472.49	kJ/mol	Joback Method
hf	-865.42	kJ/mol	Joback Method
hfus	35.05	kJ/mol	Joback Method
hvap	73.09	kJ/mol	Joback Method
log10ws	-4.62		Crippen Method
logp	3.879		Crippen Method
mcvol	243.280	ml/mol	McGowan Method
pc	1637.78	kPa	Joback Method
rinpol	1995.00		NIST Webbook
rinpol	1995.00		NIST Webbook
tb	770.99	K	Joback Method
tc	970.54	K	Joback Method
tf	435.20	K	Joback Method
vc	0.933	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	713.08	J/mol×K	770.99	Joback Method
cpg	728.35	J/mol×K	804.25	Joback Method
cpg	742.60	J/mol×K	837.51	Joback Method
cpg	755.84	J/mol×K	870.76	Joback Method
cpg	768.09	J/mol×K	904.02	Joback Method
cpg	779.35	J/mol×K	937.28	Joback Method
cpg	789.66	J/mol×K	970.54	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=U392491&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