Glutaric acid, 2-fluorophenyl 2,4-dimethylpent-3-yl ester

Inchi: InChI=1S/C18H25FO4/c1-12(2)18(13(3)4)23-17(21)11-7-10-16(20)22-15-9-6-5-8-14(15)1

InchiKey: ZSINCUDCTJHJEN-UHFFFAOYSA-N

Formula: C18H25FO4

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

Mol. weight [g/mol]: 324.39

Physical Properties

Property code	Value	Unit	Source
gf	-466.51	kJ/mol	Joback Method
hf	-891.34	kJ/mol	Joback Method
hfus	34.11	kJ/mol	Joback Method
hvap	74.93	kJ/mol	Joback Method
log10ws	-4.79		Crippen Method
logp	4.125		Crippen Method
mcvol	257.370	ml/mol	McGowan Method
pc	1527.07	kPa	Joback Method
rinpol	2082.00		NIST Webbook
rinpol	2082.00		NIST Webbook
tb	793.43	K	Joback Method
tc	994.60	K	Joback Method
tf	431.47	K	Joback Method
vc	0.984	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	770.41	J/mol×K	793.43	Joback Method
cpg	786.11	J/mol×K	826.96	Joback Method
cpg	800.72	J/mol×K	860.49	Joback Method
cpg	814.25	J/mol×K	894.02	Joback Method
cpg	826.72	J/mol×K	927.55	Joback Method
cpg	838.14	J/mol×K	961.07	Joback Method
cpg	848.54	J/mol×K	994.60	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393477&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