Glutaric acid, 2-fluorophenyl 3,7-dimethyloctyl ester

Inchi: InChI=1S/C21H31FO4/c1-16(2)8-6-9-17(3)14-15-25-20(23)12-7-13-21(24)26-19-11-5-4-1

InchiKey: FTYWCPPATJBINN-UHFFFAOYSA-N

Formula: C21H31FO4

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

Mol. weight [g/mol]: 366.47

Physical Properties

Property code	Value	Unit	Source
gf	-438.81	kJ/mol	Joback Method
hf	-947.98	kJ/mol	Joback Method
hfus	45.41	kJ/mol	Joback Method
hvap	82.00	kJ/mol	Joback Method
log10ws	-5.94		Crippen Method
logp	5.297		Crippen Method
mcvol	299.640	ml/mol	McGowan Method
pc	1226.84	kPa	Joback Method
rinpol	2458.00		NIST Webbook
rinpol	2458.00		NIST Webbook
tb	862.51	K	Joback Method
tc	1063.10	K	Joback Method
tf	480.28	K	Joback Method
vc	1.157	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	945.43	J/mol×K	862.51	Joback Method
cpg	961.59	J/mol×K	895.94	Joback Method
cpg	976.55	J/mol×K	929.37	Joback Method
cpg	990.35	J/mol×K	962.81	Joback Method
cpg	1003.00	J/mol×K	996.24	Joback Method
cpg	1014.54	J/mol×K	1029.67	Joback Method
cpg	1025.00	J/mol×K	1063.10	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=U391484&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