Glutaric acid, dec-2-yl 3-fluorophenyl ester

Inchi: InChI=1S/C21H31FO4/c1-3-4-5-6-7-8-11-17(2)25-20(23)14-10-15-21(24)26-19-13-9-12-1
InchiKey: UCLPLIRAJMUWSK-UHFFFAOYSA-N
Formula: C21H31FO4
SMILES: CCCCCCCCC(C)OC(=O)CCCC(=O)Oc1cccc(F)c1
Mol. weight [g/mol]: 366.47

Physical Properties

Property code	Value	Unit	Source
gf	-436.37	kJ/mol	Joback Method
hf	-942.70	kJ/mol	Joback Method
hfus	48.93	kJ/mol	Joback Method
hvap	82.38	kJ/mol	Joback Method
log10ws	-6.53		Crippen Method
logp	5.584		Crippen Method
mcvol	299.640	ml/mol	McGowan Method
pc	1219.99	kPa	Joback Method
rinpol	2430.00		NIST Webbook
rinpol	2430.00		NIST Webbook
tb	862.95	K	Joback Method
tc	1062.30	K	Joback Method
tf	495.28	K	Joback Method
vc	1.163	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	944.93	J/mol×K	862.95	Joback Method
cpg	961.00	J/mol×K	896.17	Joback Method
cpg	975.91	J/mol×K	929.40	Joback Method
cpg	989.67	J/mol×K	962.62	Joback Method
cpg	1002.32	J/mol×K	995.85	Joback Method
cpg	1013.87	J/mol×K	1029.07	Joback Method
cpg	1024.36	J/mol×K	1062.30	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=U392096&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