Glutaric acid, di(1-(4-fluorophenyl)ethyl) ester

Inchi: InChI=1S/C21H22F2O4/c1-14(16-6-10-18(22)11-7-16)26-20(24)4-3-5-21(25)27-15(2)17-
InchiKey: SBTQXPADMVIDSR-UHFFFAOYSA-N
Formula: C21H22F2O4
SMILES: CC(OC(=O)CCCC(=O)OC(C)c1ccc(F)cc1)c1ccc(F)cc1
Mol. weight [g/mol]: 376.39

Physical Properties

Property code	Value	Unit	Source
gf	-530.84	kJ/mol	Joback Method
hf	-919.03	kJ/mol	Joback Method
hfus	42.14	kJ/mol	Joback Method
hvap	84.12	kJ/mol	Joback Method
log10ws	-6.12		Crippen Method
logp	5.044		Crippen Method
mcvol	277.650	ml/mol	McGowan Method
pc	1497.67	kPa	Joback Method
rinpol	2489.00		NIST Webbook
rinpol	2489.00		NIST Webbook
tb	893.44	K	Joback Method
tc	1110.33	K	Joback Method
tf	519.81	K	Joback Method
vc	1.067	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	853.72	J/mol×K	893.44	Joback Method
cpg	867.20	J/mol×K	929.59	Joback Method
cpg	879.42	J/mol×K	965.74	Joback Method
cpg	890.41	J/mol×K	1001.88	Joback Method
cpg	900.19	J/mol×K	1038.03	Joback Method
cpg	908.81	J/mol×K	1074.18	Joback Method
cpg	916.30	J/mol×K	1110.33	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=U377110&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