Glutaric acid, 1-(4-fluorophenyl)ethyl 2-methylhex-3-yl ester

Inchi: InChI=1S/C20H29FO4/c1-5-7-18(14(2)3)25-20(23)9-6-8-19(22)24-15(4)16-10-12-17(21)1

InchiKey: BGSYRMLPTMUCBE-UHFFFAOYSA-N

Formula: C20H29FO4

SMILES: CCCC(OC(=O)CCCC(=O)OC(C)c1ccc(F)cc1)C(C)C

Mol. weight [g/mol]: 352.44

Physical Properties

Property code	Value	Unit	Source
gf	-449.67	kJ/mol	Joback Method
hf	-932.62	kJ/mol	Joback Method
hfus	39.29	kJ/mol	Joback Method
hvap	79.38	kJ/mol	Joback Method
log10ws	-5.68		Crippen Method
logp	4.968		Crippen Method
mcvol	285.550	ml/mol	McGowan Method
pc	1321.35	kPa	Joback Method
rinpol	2245.00		NIST Webbook
tb	839.19	K	Joback Method
tc	1040.22	K	Joback Method
tf	454.01	K	Joback Method
vc	1.095	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	886.64	J/mol×K	839.19	Joback Method
cpg	902.72	J/mol×K	872.69	Joback Method
cpg	917.62	J/mol×K	906.20	Joback Method
cpg	931.38	J/mol×K	939.70	Joback Method
cpg	944.00	J/mol×K	973.21	Joback Method
cpg	955.53	J/mol×K	1006.71	Joback Method
cpg	965.97	J/mol×K	1040.22	Joback Method

Sources

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=U377104&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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