Glutaric acid, 1,1,1-trifluoroprop-2-yl 2-isopropylphenyl ester

Inchi: InChI=1S/C17H21F3O4/c1-11(2)13-7-4-5-8-14(13)24-16(22)10-6-9-15(21)23-12(3)17(18
InchiKey: JXKGXSZVKSSUSI-UHFFFAOYSA-N
Formula: C17H21F3O4
SMILES: CC(C)c1ccccc1OC(=O)CCCC(=O)OC(C)C(F)(F)F
Mol. weight [g/mol]: 346.34

Physical Properties

Property code	Value	Unit	Source
gf	-859.27	kJ/mol	Joback Method
hf	-1266.39	kJ/mol	Joback Method
hfus	33.79	kJ/mol	Joback Method
hvap	70.16	kJ/mol	Joback Method
log10ws	-5.12		Crippen Method
logp	4.380		Crippen Method
mcvol	246.820	ml/mol	McGowan Method
pc	1547.57	kPa	Joback Method
rinpol	1833.00		NIST Webbook
rinpol	1833.00		NIST Webbook
tb	766.30	K	Joback Method
tc	961.13	K	Joback Method
tf	438.80	K	Joback Method
vc	0.959	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	730.28	J/mol×K	766.30	Joback Method
cpg	744.76	J/mol×K	798.77	Joback Method
cpg	758.25	J/mol×K	831.24	Joback Method
cpg	770.78	J/mol×K	863.72	Joback Method
cpg	782.38	J/mol×K	896.19	Joback Method
cpg	793.08	J/mol×K	928.66	Joback Method
cpg	802.92	J/mol×K	961.13	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=U391909&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