Glutaric acid, 1,1,1-trifluoroprop-2-yl 4-acetylphenyl ester

Inchi: InChI=1S/C16H17F3O5/c1-10(20)12-6-8-13(9-7-12)24-15(22)5-3-4-14(21)23-11(2)16(17

InchiKey: SKKCAXHMGOVUNQ-UHFFFAOYSA-N

Formula: C16H17F3O5

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

Mol. weight [g/mol]: 346.30

Physical Properties

Property code	Value	Unit	Source
gf	-994.17	kJ/mol	Joback Method
hf	-1353.05	kJ/mol	Joback Method
hfus	36.32	kJ/mol	Joback Method
hvap	75.07	kJ/mol	Joback Method
log10ws	-4.59		Crippen Method
logp	3.459		Crippen Method
mcvol	234.300	ml/mol	McGowan Method
pc	1749.21	kPa	Joback Method
rinpol	2083.00		NIST Webbook
rinpol	2083.00		NIST Webbook
tb	797.73	K	Joback Method
tc	998.00	K	Joback Method
tf	492.46	K	Joback Method
vc	0.914	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	689.60	J/mol×K	797.73	Joback Method
cpg	701.97	J/mol×K	831.11	Joback Method
cpg	713.38	J/mol×K	864.49	Joback Method
cpg	723.87	J/mol×K	897.86	Joback Method
cpg	733.45	J/mol×K	931.24	Joback Method
cpg	742.17	J/mol×K	964.62	Joback Method
cpg	750.05	J/mol×K	998.00	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=U392027&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