Glutaric acid, 1,1,1-trifluoroprop-2-yl 2,3,4-trifluorophenyl ester

Inchi: InChI=1S/C14H12F6O4/c1-7(14(18,19)20)23-10(21)3-2-4-11(22)24-9-6-5-8(15)12(16)13

InchiKey: ZLNAJZJIQGGMOT-UHFFFAOYSA-N

Formula: C14H12F6O4

SMILES: CC(OC(=O)CCCC(=O)Oc1ccc(F)c(F)c1F)C(F)(F)F

Mol. weight [g/mol]: 358.23

Physical Properties

Property code	Value	Unit	Source
gf	-1485.78	kJ/mol	Joback Method
hf	-1810.46	kJ/mol	Joback Method
hfus	38.01	kJ/mol	Joback Method
hvap	62.75	kJ/mol	Joback Method
log10ws	-4.93		Crippen Method
logp	3.674		Crippen Method
mcvol	209.860	ml/mol	McGowan Method
pc	1697.70	kPa	Joback Method
rinpol	1608.00		NIST Webbook
rinpol	1608.00		NIST Webbook
tb	705.87	K	Joback Method
tc	885.06	K	Joback Method
tf	446.80	K	Joback Method
vc	0.851	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	588.71	J/mol×K	705.87	Joback Method
cpg	600.30	J/mol×K	735.73	Joback Method
cpg	611.17	J/mol×K	765.60	Joback Method
cpg	621.35	J/mol×K	795.46	Joback Method
cpg	630.85	J/mol×K	825.33	Joback Method
cpg	639.68	J/mol×K	855.19	Joback Method
cpg	647.85	J/mol×K	885.06	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=U393632&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