Glutaric acid, 1,1,1-trifluoroprop-2-yl 3-fluorophenyl ester

Inchi: InChI=1S/C14H14F4O4/c1-9(14(16,17)18)21-12(19)6-3-7-13(20)22-11-5-2-4-10(15)8-11
InchiKey: QVXSXGBKWVYKBP-UHFFFAOYSA-N
Formula: C14H14F4O4
SMILES: CC(OC(=O)CCCC(=O)Oc1cccc(F)c1)C(F)(F)F
Mol. weight [g/mol]: 322.25

Physical Properties

Property code	Value	Unit	Source
gf	-1076.90	kJ/mol	Joback Method
hf	-1395.30	kJ/mol	Joback Method
hfus	32.62	kJ/mol	Joback Method
hvap	63.06	kJ/mol	Joback Method
log10ws	-4.27		Crippen Method
logp	3.395		Crippen Method
mcvol	206.320	ml/mol	McGowan Method
pc	1878.90	kPa	Joback Method
rinpol	1652.00		NIST Webbook
rinpol	1652.00		NIST Webbook
tb	697.37	K	Joback Method
tc	886.33	K	Joback Method
tf	420.58	K	Joback Method
vc	0.815	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	574.87	J/mol×K	697.37	Joback Method
cpg	587.59	J/mol×K	728.86	Joback Method
cpg	599.49	J/mol×K	760.36	Joback Method
cpg	610.58	J/mol×K	791.85	Joback Method
cpg	620.89	J/mol×K	823.34	Joback Method
cpg	630.45	J/mol×K	854.84	Joback Method
cpg	639.27	J/mol×K	886.33	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392083&Units=SI
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

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