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

Inchi: InChI=1S/C14H14ClF3O4/c1-9(14(16,17)18)21-12(19)6-3-7-13(20)22-11-5-2-4-10(15)8-1

InchiKey: WAFVEFDMCAOHFQ-UHFFFAOYSA-N

Formula: C14H14ClF3O4

SMILES: CC(OC(=O)CCCC(=O)Oc1cccc(Cl)c1)C(F)(F)F

Mol. weight [g/mol]: 338.71

Physical Properties

Property code	Value	Unit	Source
gf	-894.02	kJ/mol	Joback Method
hf	-1214.93	kJ/mol	Joback Method
hfus	33.74	kJ/mol	Joback Method
hvap	68.26	kJ/mol	Joback Method
log10ws	-4.62		Crippen Method
logp	3.910		Crippen Method
mcvol	216.790	ml/mol	McGowan Method
pc	1892.00	kPa	Joback Method
rinpol	1918.00		NIST Webbook
rinpol	1918.00		NIST Webbook
tb	735.53	K	Joback Method
tc	935.08	K	Joback Method
tf	449.91	K	Joback Method
vc	0.846	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	592.49	J/mol×K	735.53	Joback Method
cpg	604.67	J/mol×K	768.79	Joback Method
cpg	615.97	J/mol×K	802.05	Joback Method
cpg	626.42	J/mol×K	835.30	Joback Method
cpg	636.05	J/mol×K	868.56	Joback Method
cpg	644.88	J/mol×K	901.82	Joback Method
cpg	652.94	J/mol×K	935.08	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=U390453&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