Glutaric acid, 1,1,1-trifluoroprop-2-yl 2-chloro-6-fluorophenyl ester

Inchi: InChI=1S/C14H13ClF4O4/c1-8(14(17,18)19)22-11(20)6-3-7-12(21)23-13-9(15)4-2-5-10(1

InchiKey: PRBXGYPWXSINND-UHFFFAOYSA-N

Formula: C14H13ClF4O4

SMILES: CC(OC(=O)CCCC(=O)Oc1c(F)cccc1Cl)C(F)(F)F

Mol. weight [g/mol]: 356.70

Physical Properties

Property code	Value	Unit	Source
gf	-1098.46	kJ/mol	Joback Method
hf	-1422.51	kJ/mol	Joback Method
hfus	36.43	kJ/mol	Joback Method
hvap	68.10	kJ/mol	Joback Method
log10ws	-4.95		Crippen Method
logp	4.049		Crippen Method
mcvol	218.560	ml/mol	McGowan Method
pc	1796.98	kPa	Joback Method
rinpol	1788.00		NIST Webbook
rinpol	1788.00		NIST Webbook
tb	739.78	K	Joback Method
tc	933.73	K	Joback Method
tf	463.02	K	Joback Method
vc	0.864	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	599.10	J/mol×K	739.78	Joback Method
cpg	610.70	J/mol×K	772.11	Joback Method
cpg	621.49	J/mol×K	804.43	Joback Method
cpg	631.49	J/mol×K	836.76	Joback Method
cpg	640.71	J/mol×K	869.08	Joback Method
cpg	649.18	J/mol×K	901.41	Joback Method
cpg	656.92	J/mol×K	933.73	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391575&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