Glutaric acid, 1,1,1-trifluoroprop-2-yl 2,3,5-trichlorophenyl ester

Inchi: InChI=1S/C14H12Cl3F3O4/c1-7(14(18,19)20)23-11(21)3-2-4-12(22)24-10-6-8(15)5-9(16

InchiKey: QGXPYNYCSAMXKY-UHFFFAOYSA-N

Formula: C14H12Cl3F3O4

SMILES: CC(OC(=O)CCCC(=O)Oc1cc(Cl)cc(Cl)c1Cl)C(F)(F)F

Mol. weight [g/mol]: 407.60

Physical Properties

Property code	Value	Unit	Source
gf	-937.14	kJ/mol	Joback Method
hf	-1269.35	kJ/mol	Joback Method
hfus	41.36	kJ/mol	Joback Method
hvap	78.35	kJ/mol	Joback Method
log10ws	-5.99		Crippen Method
logp	5.216		Crippen Method
mcvol	241.270	ml/mol	McGowan Method
pc	1731.78	kPa	Joback Method
rinpol	2129.00		NIST Webbook
rinpol	2129.00		NIST Webbook
tb	820.35	K	Joback Method
tc	1029.25	K	Joback Method
tf	534.79	K	Joback Method
vc	0.944	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	634.96	J/mol×K	820.35	Joback Method
cpg	644.84	J/mol×K	855.17	Joback Method
cpg	653.87	J/mol×K	889.98	Joback Method
cpg	662.06	J/mol×K	924.80	Joback Method
cpg	669.44	J/mol×K	959.62	Joback Method
cpg	676.04	J/mol×K	994.43	Joback Method
cpg	681.87	J/mol×K	1029.25	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392172&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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