Glutaric acid, 1,1,1-trifluoroprop-2-yl 2,5-dichlorophenyl ester

Inchi: InChI=1S/C14H13Cl2F3O4/c1-8(14(17,18)19)22-12(20)3-2-4-13(21)23-11-7-9(15)5-6-10

InchiKey: KWXVMODILHOFQG-UHFFFAOYSA-N

Formula: C14H13Cl2F3O4

SMILES: CC(OC(=O)CCCC(=O)Oc1cc(Cl)ccc1Cl)C(F)(F)F

Mol. weight [g/mol]: 373.15

Physical Properties

Property code	Value	Unit	Source
gf	-915.58	kJ/mol	Joback Method
hf	-1242.14	kJ/mol	Joback Method
hfus	37.55	kJ/mol	Joback Method
hvap	73.30	kJ/mol	Joback Method
log10ws	-5.30		Crippen Method
logp	4.563		Crippen Method
mcvol	229.030	ml/mol	McGowan Method
pc	1809.23	kPa	Joback Method
rinpol	1977.00		NIST Webbook
rinpol	1977.00		NIST Webbook
tb	777.94	K	Joback Method
tc	982.13	K	Joback Method
tf	492.35	K	Joback Method
vc	0.894	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	614.80	J/mol×K	777.94	Joback Method
cpg	625.82	J/mol×K	811.97	Joback Method
cpg	635.97	J/mol×K	846.00	Joback Method
cpg	645.28	J/mol×K	880.04	Joback Method
cpg	653.78	J/mol×K	914.07	Joback Method
cpg	661.49	J/mol×K	948.10	Joback Method
cpg	668.44	J/mol×K	982.13	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392049&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