Glutaric acid, 2,2-dichloroethyl 2,3,4-trifluorophenyl ester

Inchi: InChI=1S/C13H11Cl2F3O4/c14-9(15)6-21-10(19)2-1-3-11(20)22-8-5-4-7(16)12(17)13(8)1

InchiKey: SXMJYYMYZPJEHY-UHFFFAOYSA-N

Formula: C13H11Cl2F3O4

SMILES: O=C(CCCC(=O)Oc1ccc(F)c(F)c1F)OCC(Cl)Cl

Mol. weight [g/mol]: 359.12

Physical Properties

Property code	Value	Unit	Source
gf	-936.47	kJ/mol	Joback Method
hf	-1224.22	kJ/mol	Joback Method
hfus	41.98	kJ/mol	Joback Method
hvap	73.04	kJ/mol	Joback Method
log10ws	-4.65		Crippen Method
logp	3.527		Crippen Method
mcvol	214.940	ml/mol	McGowan Method
pc	1908.57	kPa	Joback Method
rinpol	2063.00		NIST Webbook
rinpol	2063.00		NIST Webbook
tb	763.27	K	Joback Method
tc	962.03	K	Joback Method
tf	491.18	K	Joback Method
vc	0.850	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	558.00	J/mol×K	763.27	Joback Method
cpg	568.40	J/mol×K	796.40	Joback Method
cpg	578.04	J/mol×K	829.52	Joback Method
cpg	586.93	J/mol×K	862.65	Joback Method
cpg	595.06	J/mol×K	895.78	Joback Method
cpg	602.43	J/mol×K	928.90	Joback Method
cpg	609.04	J/mol×K	962.03	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393638&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