Glutaric acid, 3-chlorophenyl 3-fluorophenyl ester

Inchi: InChI=1S/C17H14ClFO4/c18-12-4-1-6-14(10-12)22-16(20)8-3-9-17(21)23-15-7-2-5-13(19

InchiKey: JONVYOPBAWEDTE-UHFFFAOYSA-N

Formula: C17H14ClFO4

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

Mol. weight [g/mol]: 336.74

Physical Properties

Property code	Value	Unit	Source
gf	-376.76	kJ/mol	Joback Method
hf	-645.54	kJ/mol	Joback Method
hfus	39.94	kJ/mol	Joback Method
hvap	81.19	kJ/mol	Joback Method
log10ws	-5.18		Crippen Method
logp	4.160		Crippen Method
mcvol	231.760	ml/mol	McGowan Method
pc	2051.17	kPa	Joback Method
rinpol	2457.00		NIST Webbook
rinpol	2457.00		NIST Webbook
tb	840.96	K	Joback Method
tc	1068.17	K	Joback Method
tf	534.06	K	Joback Method
vc	0.886	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	641.78	J/mol×K	840.96	Joback Method
cpg	653.54	J/mol×K	878.83	Joback Method
cpg	664.15	J/mol×K	916.70	Joback Method
cpg	673.66	J/mol×K	954.56	Joback Method
cpg	682.07	J/mol×K	992.43	Joback Method
cpg	689.42	J/mol×K	1030.30	Joback Method
cpg	695.73	J/mol×K	1068.17	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392095&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