Glutaric acid, 2-chloro-6-fluorophenyl 3-fluorophenyl ester

Inchi: InChI=1S/C17H13ClF2O4/c18-13-6-2-7-14(20)17(13)24-16(22)9-3-8-15(21)23-12-5-1-4-1

InchiKey: URHXPFSRNFTWCJ-UHFFFAOYSA-N

Formula: C17H13ClF2O4

SMILES: O=C(CCCC(=O)Oc1c(F)cccc1Cl)Oc1cccc(F)c1

Mol. weight [g/mol]: 354.73

Physical Properties

Property code	Value	Unit	Source
gf	-581.20	kJ/mol	Joback Method
hf	-853.12	kJ/mol	Joback Method
hfus	42.63	kJ/mol	Joback Method
hvap	81.04	kJ/mol	Joback Method
log10ws	-5.51		Crippen Method
logp	4.300		Crippen Method
mcvol	233.530	ml/mol	McGowan Method
pc	1944.08	kPa	Joback Method
rinpol	2403.00		NIST Webbook
rinpol	2403.00		NIST Webbook
tb	845.21	K	Joback Method
tc	1065.97	K	Joback Method
tf	547.17	K	Joback Method
vc	0.904	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	647.75	J/mol×K	845.21	Joback Method
cpg	658.94	J/mol×K	882.00	Joback Method
cpg	669.05	J/mol×K	918.80	Joback Method
cpg	678.11	J/mol×K	955.59	Joback Method
cpg	686.12	J/mol×K	992.38	Joback Method
cpg	693.11	J/mol×K	1029.17	Joback Method
cpg	699.10	J/mol×K	1065.97	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392094&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