Glutaric acid, di(2-chloro-6-fluorophenyl) ester

Inchi: InChI=1S/C17H12Cl2F2O4/c18-10-4-1-6-12(20)16(10)24-14(22)8-3-9-15(23)25-17-11(19
InchiKey: INVHZKBJVAZCKA-UHFFFAOYSA-N
Formula: C17H12Cl2F2O4
SMILES: O=C(CCCC(=O)Oc1c(F)cccc1Cl)Oc1c(F)cccc1Cl
Mol. weight [g/mol]: 389.18

Physical Properties

Property code	Value	Unit	Source
gf	-602.76	kJ/mol	Joback Method
hf	-880.33	kJ/mol	Joback Method
hfus	46.44	kJ/mol	Joback Method
hvap	86.08	kJ/mol	Joback Method
log10ws	-6.20		Crippen Method
logp	4.953		Crippen Method
mcvol	245.770	ml/mol	McGowan Method
pc	1857.91	kPa	Joback Method
rinpol	2560.00		NIST Webbook
rinpol	2560.00		NIST Webbook
tb	887.62	K	Joback Method
tc	1112.64	K	Joback Method
tf	589.61	K	Joback Method
vc	0.954	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	666.59	J/mol×K	887.62	Joback Method
cpg	676.45	J/mol×K	925.12	Joback Method
cpg	685.22	J/mol×K	962.63	Joback Method
cpg	692.91	J/mol×K	1000.13	Joback Method
cpg	699.54	J/mol×K	1037.63	Joback Method
cpg	705.12	J/mol×K	1075.13	Joback Method
cpg	709.67	J/mol×K	1112.64	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391593&Units=SI

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