Glutaric acid, 2-chloro-6-fluorophenyl 2-methyl-4-chlorophenyl ester

Inchi: InChI=1S/C18H15Cl2FO4/c1-11-10-12(19)8-9-15(11)24-16(22)6-3-7-17(23)25-18-13(20)
InchiKey: YLZKWIYNLFAVRP-UHFFFAOYSA-N
Formula: C18H15Cl2FO4
SMILES: Cc1cc(Cl)ccc1OC(=O)CCCC(=O)Oc1c(F)cccc1Cl
Mol. weight [g/mol]: 385.21

Physical Properties

Property code	Value	Unit	Source
gf	-399.53	kJ/mol	Joback Method
hf	-704.86	kJ/mol	Joback Method
hfus	45.95	kJ/mol	Joback Method
hvap	89.13	kJ/mol	Joback Method
log10ws	-6.34		Crippen Method
logp	5.122		Crippen Method
mcvol	258.090	ml/mol	McGowan Method
pc	1778.84	kPa	Joback Method
rinpol	2734.00		NIST Webbook
rinpol	2734.00		NIST Webbook
tb	911.23	K	Joback Method
tc	1141.06	K	Joback Method
tf	600.29	K	Joback Method
vc	0.992	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	714.97	J/mol×K	911.23	Joback Method
cpg	725.43	J/mol×K	949.54	Joback Method
cpg	734.70	J/mol×K	987.84	Joback Method
cpg	742.81	J/mol×K	1026.15	Joback Method
cpg	749.76	J/mol×K	1064.45	Joback Method
cpg	755.58	J/mol×K	1102.76	Joback Method
cpg	760.28	J/mol×K	1141.06	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=U392074&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