Glutaric acid, 2-chloro-6-fluorophenyl 2,3,4-trifluorophenyl ester

Inchi: InChI=1S/C17H11ClF4O4/c18-9-3-1-4-11(20)17(9)26-14(24)6-2-5-13(23)25-12-8-7-10(19

InchiKey: BOJCZGLIVUGGEU-UHFFFAOYSA-N

Formula: C17H11ClF4O4

SMILES: O=C(CCCC(=O)Oc1c(F)cccc1Cl)Oc1ccc(F)c(F)c1F

Mol. weight [g/mol]: 390.71

Physical Properties

Property code	Value	Unit	Source
gf	-990.08	kJ/mol	Joback Method
hf	-1268.28	kJ/mol	Joback Method
hfus	48.01	kJ/mol	Joback Method
hvap	80.73	kJ/mol	Joback Method
log10ws	-6.18		Crippen Method
logp	4.578		Crippen Method
mcvol	237.070	ml/mol	McGowan Method
pc	1753.60	kPa	Joback Method
rinpol	2354.00		NIST Webbook
rinpol	2354.00		NIST Webbook
tb	853.71	K	Joback Method
tc	1064.00	K	Joback Method
tf	573.39	K	Joback Method
vc	0.941	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	659.57	J/mol×K	853.71	Joback Method
cpg	669.77	J/mol×K	888.76	Joback Method
cpg	679.00	J/mol×K	923.81	Joback Method
cpg	687.25	J/mol×K	958.86	Joback Method
cpg	694.54	J/mol×K	993.90	Joback Method
cpg	700.87	J/mol×K	1028.95	Joback Method
cpg	706.24	J/mol×K	1064.00	Joback Method

Sources

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=U393642&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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