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

Inchi: InChI=1S/C18H24ClFO4/c1-4-7-15(12(2)3)23-16(21)10-6-11-17(22)24-18-13(19)8-5-9-14

InchiKey: RSAWJSWCBKNRLN-UHFFFAOYSA-N

Formula: C18H24ClFO4

SMILES: CCCC(OC(=O)CCCC(=O)Oc1c(F)cccc1Cl)C(C)C

Mol. weight [g/mol]: 358.83

Physical Properties

Property code	Value	Unit	Source
gf	-485.63	kJ/mol	Joback Method
hf	-913.27	kJ/mol	Joback Method
hfus	41.44	kJ/mol	Joback Method
hvap	80.37	kJ/mol	Joback Method
log10ws	-5.72		Crippen Method
logp	4.923		Crippen Method
mcvol	269.610	ml/mol	McGowan Method
pc	1457.90	kPa	Joback Method
rinpol	2223.00		NIST Webbook
rinpol	2223.00		NIST Webbook
tb	836.28	K	Joback Method
tc	1040.45	K	Joback Method
tf	488.91	K	Joback Method
vc	1.038	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	795.98	J/mol×K	836.28	Joback Method
cpg	810.25	J/mol×K	870.31	Joback Method
cpg	823.43	J/mol×K	904.34	Joback Method
cpg	835.54	J/mol×K	938.37	Joback Method
cpg	846.60	J/mol×K	972.40	Joback Method
cpg	856.63	J/mol×K	1006.42	Joback Method
cpg	865.63	J/mol×K	1040.45	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393735&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