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

Inchi: InChI=1S/C19H24ClFO4/c1-2-13-7-3-4-10-16(13)24-17(22)11-6-12-18(23)25-19-14(20)8

InchiKey: GSXFJQRWAQKVPX-UHFFFAOYSA-N

Formula: C19H24ClFO4

SMILES: CCC1CCCCC1OC(=O)CCCC(=O)Oc1c(F)cccc1Cl

Mol. weight [g/mol]: 370.84

Physical Properties

Property code	Value	Unit	Source
gf	-455.59	kJ/mol	Joback Method
hf	-889.37	kJ/mol	Joback Method
hfus	43.99	kJ/mol	Joback Method
hvap	83.49	kJ/mol	Joback Method
log10ws	-6.03		Crippen Method
logp	5.067		Crippen Method
mcvol	272.840	ml/mol	McGowan Method
pc	1527.07	kPa	Joback Method
rinpol	2477.00		NIST Webbook
rinpol	2477.00		NIST Webbook
tb	874.92	K	Joback Method
tc	1093.67	K	Joback Method
tf	533.32	K	Joback Method
vc	1.038	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	851.13	J/mol×K	874.92	Joback Method
cpg	866.28	J/mol×K	911.38	Joback Method
cpg	879.97	J/mol×K	947.84	Joback Method
cpg	892.23	J/mol×K	984.30	Joback Method
cpg	903.05	J/mol×K	1020.75	Joback Method
cpg	912.47	J/mol×K	1057.21	Joback Method
cpg	920.50	J/mol×K	1093.67	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=U405480&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