Glutaric acid, oct-1-en-3-yl 2-chloro-6-fluorophenyl ester

Inchi: InChI=1S/C19H24ClFO4/c1-3-5-6-9-14(4-2)24-17(22)12-8-13-18(23)25-19-15(20)10-7-11

InchiKey: YAMQJZIDTSVEIP-UHFFFAOYSA-N

Formula: C19H24ClFO4

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

Mol. weight [g/mol]: 370.84

Physical Properties

Property code	Value	Unit	Source
gf	-386.93	kJ/mol	Joback Method
hf	-803.20	kJ/mol	Joback Method
hfus	46.28	kJ/mol	Joback Method
hvap	82.31	kJ/mol	Joback Method
log10ws	-6.23		Crippen Method
logp	5.233		Crippen Method
mcvol	279.400	ml/mol	McGowan Method
pc	1391.25	kPa	Joback Method
rinpol	2363.00		NIST Webbook
rinpol	2363.00		NIST Webbook
tb	856.28	K	Joback Method
tc	1060.49	K	Joback Method
tf	513.42	K	Joback Method
vc	1.081	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	825.79	J/mol×K	856.28	Joback Method
cpg	839.69	J/mol×K	890.32	Joback Method
cpg	852.52	J/mol×K	924.35	Joback Method
cpg	864.32	J/mol×K	958.39	Joback Method
cpg	875.09	J/mol×K	992.42	Joback Method
cpg	884.88	J/mol×K	1026.46	Joback Method
cpg	893.69	J/mol×K	1060.49	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405353&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