Glutaric acid, hexa-1,5-dien-3-yl 2-chloro-6-fluorophenyl ester

Inchi: InChI=1S/C17H18ClFO4/c1-3-7-12(4-2)22-15(20)10-6-11-16(21)23-17-13(18)8-5-9-14(1

InchiKey: SYZFUGYGSFNRCC-UHFFFAOYSA-N

Formula: C17H18ClFO4

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

Mol. weight [g/mol]: 340.77

Physical Properties

Property code	Value	Unit	Source
gf	-315.93	kJ/mol	Joback Method
hf	-636.49	kJ/mol	Joback Method
hfus	39.82	kJ/mol	Joback Method
hvap	77.19	kJ/mol	Joback Method
log10ws	-5.25		Crippen Method
logp	4.229		Crippen Method
mcvol	246.920	ml/mol	McGowan Method
pc	1670.06	kPa	Joback Method
rinpol	2148.00		NIST Webbook
rinpol	2148.00		NIST Webbook
tb	807.20	K	Joback Method
tc	1013.76	K	Joback Method
tf	489.12	K	Joback Method
vc	0.951	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	685.74	J/mol×K	807.20	Joback Method
cpg	698.58	J/mol×K	841.63	Joback Method
cpg	710.46	J/mol×K	876.05	Joback Method
cpg	721.40	J/mol×K	910.48	Joback Method
cpg	731.44	J/mol×K	944.91	Joback Method
cpg	740.59	J/mol×K	979.33	Joback Method
cpg	748.87	J/mol×K	1013.76	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=U405283&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