Glutaric acid, 2-chloro-6-fluorophenyl cis-hex-3-enyl ester

Inchi: InChI=1S/C17H20ClFO4/c1-2-3-4-5-12-22-15(20)10-7-11-16(21)23-17-13(18)8-6-9-14(1
InchiKey: SDYCUMFRKNWNIE-ARJAWSKDSA-N
Formula: C17H20ClFO4
SMILES: CCC=CCCOC(=O)CCCC(=O)Oc1c(F)cccc1Cl
Mol. weight [g/mol]: 342.79

Physical Properties

Property code	Value	Unit	Source
gf	-408.95	kJ/mol	Joback Method
hf	-764.85	kJ/mol	Joback Method
hfus	46.10	kJ/mol	Joback Method
hvap	78.87	kJ/mol	Joback Method
log10ws	-5.29		Crippen Method
logp	4.454		Crippen Method
mcvol	251.220	ml/mol	McGowan Method
pc	1616.77	kPa	Joback Method
rinpol	2318.00		NIST Webbook
rinpol	2318.00		NIST Webbook
tb	818.44	K	Joback Method
tc	1023.34	K	Joback Method
tf	502.56	K	Joback Method
vc	0.975	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	711.69	J/mol×K	818.44	Joback Method
cpg	724.91	J/mol×K	852.59	Joback Method
cpg	737.20	J/mol×K	886.74	Joback Method
cpg	748.57	J/mol×K	920.89	Joback Method
cpg	759.06	J/mol×K	955.04	Joback Method
cpg	768.69	J/mol×K	989.19	Joback Method
cpg	777.48	J/mol×K	1023.34	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=U394029&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