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

Inchi: InChI=1S/C15H16ClFO4/c1-2-3-10-20-13(18)8-5-9-14(19)21-15-11(16)6-4-7-12(15)17/h2

InchiKey: WHRXVOGXXMQMBB-UHFFFAOYSA-N

Formula: C15H16ClFO4

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

Mol. weight [g/mol]: 314.74

Physical Properties

Property code	Value	Unit	Source
gf	-418.17	kJ/mol	Joback Method
hf	-715.36	kJ/mol	Joback Method
hfus	39.44	kJ/mol	Joback Method
hvap	73.79	kJ/mol	Joback Method
log10ws	-4.45		Crippen Method
logp	3.674		Crippen Method
mcvol	223.040	ml/mol	McGowan Method
pc	1882.17	kPa	Joback Method
rinpol	2082.00		NIST Webbook
rinpol	2082.00		NIST Webbook
tb	765.20	K	Joback Method
tc	969.16	K	Joback Method
tf	483.34	K	Joback Method
vc	0.864	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	601.41	J/mol×K	765.20	Joback Method
cpg	613.92	J/mol×K	799.19	Joback Method
cpg	625.56	J/mol×K	833.19	Joback Method
cpg	636.34	J/mol×K	867.18	Joback Method
cpg	646.28	J/mol×K	901.17	Joback Method
cpg	655.38	J/mol×K	935.17	Joback Method
cpg	663.65	J/mol×K	969.16	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U394040&Units=SI

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

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