Glutaric acid, 2-chloro-6-fluorophenyl 3-methylbutyl ester

Inchi: InChI=1S/C16H20ClFO4/c1-11(2)9-10-21-14(19)7-4-8-15(20)22-16-12(17)5-3-6-13(16)18

InchiKey: VJHMOHZHMOHVJQ-UHFFFAOYSA-N

Formula: C16H20ClFO4

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

Mol. weight [g/mol]: 330.78

Physical Properties

Property code	Value	Unit	Source
gf	-500.03	kJ/mol	Joback Method
hf	-866.71	kJ/mol	Joback Method
hfus	39.79	kJ/mol	Joback Method
hvap	76.30	kJ/mol	Joback Method
log10ws	-4.77		Crippen Method
logp	4.144		Crippen Method
mcvol	241.430	ml/mol	McGowan Method
pc	1686.56	kPa	Joback Method
rinpol	2329.00		NIST Webbook
rinpol	2329.00		NIST Webbook
tb	790.96	K	Joback Method
tc	993.83	K	Joback Method
tf	481.37	K	Joback Method
vc	0.932	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	682.35	J/mol×K	790.96	Joback Method
cpg	695.94	J/mol×K	824.77	Joback Method
cpg	708.56	J/mol×K	858.58	Joback Method
cpg	720.22	J/mol×K	892.40	Joback Method
cpg	730.94	J/mol×K	926.21	Joback Method
cpg	740.72	J/mol×K	960.02	Joback Method
cpg	749.58	J/mol×K	993.83	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=U391441&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