Glutaric acid, 3-methylbut-2-yl 2-chloro-6-fluorophenyl ester

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

InchiKey: AQYDVOHHCOSRMD-UHFFFAOYSA-N

Formula: C16H20ClFO4

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

Mol. weight [g/mol]: 330.78

Physical Properties

Property code	Value	Unit	Source
gf	-502.47	kJ/mol	Joback Method
hf	-871.99	kJ/mol	Joback Method
hfus	36.26	kJ/mol	Joback Method
hvap	75.91	kJ/mol	Joback Method
log10ws	-4.88		Crippen Method
logp	4.142		Crippen Method
mcvol	241.430	ml/mol	McGowan Method
pc	1697.70	kPa	Joback Method
rinpol	2082.00		NIST Webbook
rinpol	2082.00		NIST Webbook
tb	790.52	K	Joback Method
tc	995.99	K	Joback Method
tf	466.37	K	Joback Method
vc	0.926	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	682.92	J/mol×K	790.52	Joback Method
cpg	696.68	J/mol×K	824.77	Joback Method
cpg	709.43	J/mol×K	859.01	Joback Method
cpg	721.20	J/mol×K	893.26	Joback Method
cpg	731.99	J/mol×K	927.50	Joback Method
cpg	741.80	J/mol×K	961.75	Joback Method
cpg	750.66	J/mol×K	995.99	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391579&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

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