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

Inchi: InChI=1S/C20H20ClFO4/c21-16-10-4-11-17(22)20(16)26-19(24)13-5-12-18(23)25-14-6-9

InchiKey: PKVPAXNRGREWKL-UHFFFAOYSA-N

Formula: C20H20ClFO4

SMILES: O=C(CCCC(=O)Oc1c(F)cccc1Cl)OCCCc1ccccc1

Mol. weight [g/mol]: 378.82

Physical Properties

Property code	Value	Unit	Source
gf	-351.50	kJ/mol	Joback Method
hf	-707.46	kJ/mol	Joback Method
hfus	47.71	kJ/mol	Joback Method
hvap	87.87	kJ/mol	Joback Method
log10ws	-5.79		Crippen Method
logp	4.731		Crippen Method
mcvol	274.030	ml/mol	McGowan Method
pc	1605.13	kPa	Joback Method
rinpol	2768.00		NIST Webbook
rinpol	2768.00		NIST Webbook
tb	909.60	K	Joback Method
tc	1131.97	K	Joback Method
tf	567.87	K	Joback Method
vc	1.054	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	810.60	J/mol×K	909.60	Joback Method
cpg	822.87	J/mol×K	946.66	Joback Method
cpg	833.92	J/mol×K	983.72	Joback Method
cpg	843.79	J/mol×K	1020.78	Joback Method
cpg	852.50	J/mol×K	1057.84	Joback Method
cpg	860.11	J/mol×K	1094.90	Joback Method
cpg	866.64	J/mol×K	1131.97	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=U391778&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