Glutaric acid, 2-chloro-6-fluorophenyl 2-propylphenyl ester

Inchi: InChI=1S/C20H20ClFO4/c1-2-7-14-8-3-4-11-17(14)25-18(23)12-6-13-19(24)26-20-15(21
InchiKey: ATTZEQBVDLLULU-UHFFFAOYSA-N
Formula: C20H20ClFO4
SMILES: CCCc1ccccc1OC(=O)CCCC(=O)Oc1c(F)cccc1Cl
Mol. weight [g/mol]: 378.82

Physical Properties

Property code	Value	Unit	Source
gf	-361.13	kJ/mol	Joback Method
hf	-718.93	kJ/mol	Joback Method
hfus	47.32	kJ/mol	Joback Method
hvap	88.53	kJ/mol	Joback Method
log10ws	-6.40		Crippen Method
logp	5.113		Crippen Method
mcvol	274.030	ml/mol	McGowan Method
pc	1586.01	kPa	Joback Method
rinpol	2638.00		NIST Webbook
rinpol	2638.00		NIST Webbook
tb	914.58	K	Joback Method
tc	1137.74	K	Joback Method
tf	580.39	K	Joback Method
vc	1.054	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	809.25	J/mol×K	914.58	Joback Method
cpg	821.41	J/mol×K	951.77	Joback Method
cpg	832.35	J/mol×K	988.97	Joback Method
cpg	842.07	J/mol×K	1026.16	Joback Method
cpg	850.62	J/mol×K	1063.35	Joback Method
cpg	858.02	J/mol×K	1100.55	Joback Method
cpg	864.30	J/mol×K	1137.74	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392145&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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