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

Inchi: InChI=1S/C21H30ClFO4/c1-3-4-5-6-7-8-11-16(2)26-19(24)14-10-15-20(25)27-21-17(22)
InchiKey: GCEWDRIIEUHUPL-UHFFFAOYSA-N
Formula: C21H30ClFO4
SMILES: CCCCCCCCC(C)OC(=O)CCCC(=O)Oc1c(F)cccc1Cl
Mol. weight [g/mol]: 400.91

Physical Properties

Property code	Value	Unit	Source
gf	-457.93	kJ/mol	Joback Method
hf	-969.91	kJ/mol	Joback Method
hfus	52.74	kJ/mol	Joback Method
hvap	87.43	kJ/mol	Joback Method
log10ws	-7.22		Crippen Method
logp	6.237		Crippen Method
mcvol	311.880	ml/mol	McGowan Method
pc	1176.85	kPa	Joback Method
rinpol	2573.00		NIST Webbook
rinpol	2573.00		NIST Webbook
tb	905.36	K	Joback Method
tc	1111.84	K	Joback Method
tf	537.72	K	Joback Method
vc	1.212	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	971.15	J/mol×K	905.36	Joback Method
cpg	985.99	J/mol×K	939.77	Joback Method
cpg	999.61	J/mol×K	974.19	Joback Method
cpg	1012.05	J/mol×K	1008.60	Joback Method
cpg	1023.32	J/mol×K	1043.02	Joback Method
cpg	1033.46	J/mol×K	1077.43	Joback Method
cpg	1042.48	J/mol×K	1111.84	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393511&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