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

Inchi: InChI=1S/C21H30ClFO4/c1-2-3-4-5-6-7-8-9-16-26-19(24)14-11-15-20(25)27-21-17(22)12
InchiKey: XEVLQXRVPDHNQI-UHFFFAOYSA-N
Formula: C21H30ClFO4
SMILES: CCCCCCCCCCOC(=O)CCCC(=O)Oc1c(F)cccc1Cl
Mol. weight [g/mol]: 400.91

Physical Properties

Property code	Value	Unit	Source
gf	-455.49	kJ/mol	Joback Method
hf	-964.63	kJ/mol	Joback Method
hfus	56.26	kJ/mol	Joback Method
hvap	87.82	kJ/mol	Joback Method
log10ws	-7.11		Crippen Method
logp	6.239		Crippen Method
mcvol	311.880	ml/mol	McGowan Method
pc	1170.42	kPa	Joback Method
rinpol	2716.00		NIST Webbook
rinpol	2716.00		NIST Webbook
tb	905.80	K	Joback Method
tc	1111.46	K	Joback Method
tf	552.72	K	Joback Method
vc	1.218	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	970.66	J/mol×K	905.80	Joback Method
cpg	985.47	J/mol×K	940.08	Joback Method
cpg	999.09	J/mol×K	974.35	Joback Method
cpg	1011.54	J/mol×K	1008.63	Joback Method
cpg	1022.84	J/mol×K	1042.91	Joback Method
cpg	1033.03	J/mol×K	1077.18	Joback Method
cpg	1042.13	J/mol×K	1111.46	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=U391550&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