Glutaric acid, 2-fluorophenyl 10-chlorodecyl ester

Inchi: InChI=1S/C21H30ClFO4/c22-16-9-5-3-1-2-4-6-10-17-26-20(24)14-11-15-21(25)27-19-13

InchiKey: CTINSQNLZTYWBE-UHFFFAOYSA-N

Formula: C21H30ClFO4

SMILES: O=C(CCCC(=O)Oc1ccccc1F)OCCCCCCCCCCCCl

Mol. weight [g/mol]: 400.91

Physical Properties

Property code	Value	Unit	Source
gf	-445.86	kJ/mol	Joback Method
hf	-953.16	kJ/mol	Joback Method
hfus	56.65	kJ/mol	Joback Method
hvap	87.16	kJ/mol	Joback Method
log10ws	-6.57		Crippen Method
logp	5.804		Crippen Method
mcvol	311.880	ml/mol	McGowan Method
pc	1182.53	kPa	Joback Method
rinpol	2892.00		NIST Webbook
rinpol	2892.00		NIST Webbook
tb	900.82	K	Joback Method
tc	1105.50	K	Joback Method
tf	540.20	K	Joback Method
vc	1.218	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	971.49	J/mol×K	900.82	Joback Method
cpg	986.38	J/mol×K	934.93	Joback Method
cpg	1000.10	J/mol×K	969.05	Joback Method
cpg	1012.67	J/mol×K	1003.16	Joback Method
cpg	1024.12	J/mol×K	1037.27	Joback Method
cpg	1034.48	J/mol×K	1071.39	Joback Method
cpg	1043.79	J/mol×K	1105.50	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=U392466&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