Glutaric acid, 2-chloro-6-fluorophenyl 10-chlorodecyl ester

Inchi: InChI=1S/C21H29Cl2FO4/c22-15-7-5-3-1-2-4-6-8-16-27-19(25)13-10-14-20(26)28-21-17

InchiKey: UBMNAFWUIRSFLG-UHFFFAOYSA-N

Formula: C21H29Cl2FO4

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

Mol. weight [g/mol]: 435.36

Physical Properties

Property code	Value	Unit	Source
gf	-467.42	kJ/mol	Joback Method
hf	-980.37	kJ/mol	Joback Method
hfus	60.46	kJ/mol	Joback Method
hvap	92.20	kJ/mol	Joback Method
log10ws	-7.26		Crippen Method
logp	6.458		Crippen Method
mcvol	324.120	ml/mol	McGowan Method
pc	1141.34	kPa	Joback Method
rinpol	3039.00		NIST Webbook
rinpol	3039.00		NIST Webbook
tb	943.23	K	Joback Method
tc	1155.86	K	Joback Method
tf	582.64	K	Joback Method
vc	1.268	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	995.46	J/mol×K	943.23	Joback Method
cpg	1009.14	J/mol×K	978.67	Joback Method
cpg	1021.59	J/mol×K	1014.11	Joback Method
cpg	1032.84	J/mol×K	1049.54	Joback Method
cpg	1042.92	J/mol×K	1084.98	Joback Method
cpg	1051.86	J/mol×K	1120.42	Joback Method
cpg	1059.69	J/mol×K	1155.86	Joback Method

Sources

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=U392469&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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