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

Inchi: InChI=1S/C17H9Cl6FO4/c18-7-3-1-4-8(24)16(7)27-9(25)5-2-6-10(26)28-17-14(22)12(20)

InchiKey: XIYMPCNLPCASBA-UHFFFAOYSA-N

Formula: C17H9Cl6FO4

SMILES: O=C(CCCC(=O)Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl)Oc1c(F)cccc1Cl

Mol. weight [g/mol]: 508.97

Physical Properties

Property code	Value	Unit	Source
gf	-484.56	kJ/mol	Joback Method
hf	-781.59	kJ/mol	Joback Method
hfus	58.98	kJ/mol	Joback Method
hvap	106.43	kJ/mol	Joback Method
log10ws	-8.61		Crippen Method
logp	7.427		Crippen Method
mcvol	292.960	ml/mol	McGowan Method
pc	1641.76	kPa	Joback Method
rinpol	3185.00		NIST Webbook
rinpol	3185.00		NIST Webbook
tb	1053.01	K	Joback Method
tc	1301.75	K	Joback Method
tf	746.26	K	Joback Method
vc	1.131	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	717.56	J/mol×K	1053.01	Joback Method
cpg	722.19	J/mol×K	1094.47	Joback Method
cpg	725.53	J/mol×K	1135.92	Joback Method
cpg	727.58	J/mol×K	1177.38	Joback Method
cpg	728.35	J/mol×K	1218.83	Joback Method
cpg	727.83	J/mol×K	1260.29	Joback Method
cpg	726.02	J/mol×K	1301.75	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392205&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