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

Inchi: InChI=1S/C17H9ClF6O4/c18-7-3-1-4-8(19)16(7)27-9(25)5-2-6-10(26)28-17-14(23)12(21)
InchiKey: MQBRQMXPKVCTCG-UHFFFAOYSA-N
Formula: C17H9ClF6O4
SMILES: O=C(CCCC(=O)Oc1c(F)c(F)c(F)c(F)c1F)Oc1c(F)cccc1Cl
Mol. weight [g/mol]: 426.69

Physical Properties

Property code	Value	Unit	Source
gf	-1398.96	kJ/mol	Joback Method
hf	-1683.44	kJ/mol	Joback Method
hfus	53.40	kJ/mol	Joback Method
hvap	80.42	kJ/mol	Joback Method
log10ws	-6.84		Crippen Method
logp	4.856		Crippen Method
mcvol	240.610	ml/mol	McGowan Method
pc	1589.81	kPa	Joback Method
rinpol	2177.00		NIST Webbook
rinpol	2177.00		NIST Webbook
tb	862.21	K	Joback Method
tc	1065.19	K	Joback Method
tf	599.61	K	Joback Method
vc	0.977	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	671.21	J/mol×K	862.21	Joback Method
cpg	680.61	J/mol×K	896.04	Joback Method
cpg	689.10	J/mol×K	929.87	Joback Method
cpg	696.68	J/mol×K	963.70	Joback Method
cpg	703.32	J/mol×K	997.53	Joback Method
cpg	709.04	J/mol×K	1031.36	Joback Method
cpg	713.83	J/mol×K	1065.19	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=U392111&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