Glutaric acid, 2-chloro-6-fluorophenyl 4-biphenyl ester

Inchi: InChI=1S/C23H18ClFO4/c24-19-8-4-9-20(25)23(19)29-22(27)11-5-10-21(26)28-18-14-12

InchiKey: GFNVBNFYJWTFFI-UHFFFAOYSA-N

Formula: C23H18ClFO4

SMILES: O=C(CCCC(=O)Oc1c(F)cccc1Cl)Oc1ccc(-c2ccccc2)cc1

Mol. weight [g/mol]: 412.84

Physical Properties

Property code	Value	Unit	Source
gf	-223.46	kJ/mol	Joback Method
hf	-544.32	kJ/mol	Joback Method
hfus	49.13	kJ/mol	Joback Method
hvap	97.49	kJ/mol	Joback Method
log10ws	-7.79		Crippen Method
logp	5.827		Crippen Method
mcvol	292.540	ml/mol	McGowan Method
pc	1641.76	kPa	Joback Method
rinpol	3263.00		NIST Webbook
rinpol	3263.00		NIST Webbook
tb	1009.90	K	Joback Method
tc	1255.13	K	Joback Method
tf	640.62	K	Joback Method
vc	1.115	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	874.22	J/mol×K	1009.90	Joback Method
cpg	884.13	J/mol×K	1050.77	Joback Method
cpg	892.64	J/mol×K	1091.64	Joback Method
cpg	899.80	J/mol×K	1132.51	Joback Method
cpg	905.68	J/mol×K	1173.39	Joback Method
cpg	910.34	J/mol×K	1214.26	Joback Method
cpg	913.84	J/mol×K	1255.13	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390127&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