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

Inchi: InChI=1S/C18H13ClFNO4/c19-14-3-1-4-15(20)18(14)25-17(23)6-2-5-16(22)24-13-9-7-12

InchiKey: IKVNSRPJOGXNDK-UHFFFAOYSA-N

Formula: C18H13ClFNO4

SMILES: N#Cc1ccc(OC(=O)CCCC(=O)Oc2c(F)cccc2Cl)cc1

Mol. weight [g/mol]: 361.75

Physical Properties

Property code	Value	Unit	Source
gf	-244.79	kJ/mol	Joback Method
hf	-512.77	kJ/mol	Joback Method
hfus	43.65	kJ/mol	Joback Method
hvap	94.56	kJ/mol	Joback Method
log10ws	-5.54		Crippen Method
logp	4.032		Crippen Method
mcvol	247.230	ml/mol	McGowan Method
pc	1820.06	kPa	Joback Method
rinpol	2823.00		NIST Webbook
rinpol	2823.00		NIST Webbook
tb	970.90	K	Joback Method
tc	1208.60	K	Joback Method
tf	622.84	K	Joback Method
vc	0.969	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	702.45	J/mol×K	970.90	Joback Method
cpg	710.74	J/mol×K	1010.52	Joback Method
cpg	717.83	J/mol×K	1050.13	Joback Method
cpg	723.75	J/mol×K	1089.75	Joback Method
cpg	728.51	J/mol×K	1129.37	Joback Method
cpg	732.15	J/mol×K	1168.98	Joback Method
cpg	734.68	J/mol×K	1208.60	Joback Method

Sources

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=U393277&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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