Glutaric acid, 3-chlorophenyl 4-cyanophenyl ester

Inchi: InChI=1S/C18H14ClNO4/c19-14-3-1-4-16(11-14)24-18(22)6-2-5-17(21)23-15-9-7-13(12-

InchiKey: QPXWOKARMRSKFW-UHFFFAOYSA-N

Formula: C18H14ClNO4

SMILES: N#Cc1ccc(OC(=O)CCCC(=O)Oc2cccc(Cl)c2)cc1

Mol. weight [g/mol]: 343.76

Physical Properties

Property code	Value	Unit	Source
gf	-40.35	kJ/mol	Joback Method
hf	-305.19	kJ/mol	Joback Method
hfus	40.96	kJ/mol	Joback Method
hvap	94.71	kJ/mol	Joback Method
log10ws	-5.20		Crippen Method
logp	3.893		Crippen Method
mcvol	245.460	ml/mol	McGowan Method
pc	1916.94	kPa	Joback Method
rinpol	2880.00		NIST Webbook
rinpol	2880.00		NIST Webbook
tb	966.65	K	Joback Method
tc	1209.77	K	Joback Method
tf	609.73	K	Joback Method
vc	0.951	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	697.32	J/mol×K	966.65	Joback Method
cpg	706.08	J/mol×K	1007.17	Joback Method
cpg	713.62	J/mol×K	1047.69	Joback Method
cpg	719.96	J/mol×K	1088.21	Joback Method
cpg	725.13	J/mol×K	1128.73	Joback Method
cpg	729.17	J/mol×K	1169.25	Joback Method
cpg	732.11	J/mol×K	1209.77	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393278&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