Glutaric acid, 2,4,6-trichlorophenyl 2-nitrophenyl ester

Inchi: InChI=1S/C17H12Cl3NO6/c18-10-8-11(19)17(12(20)9-10)27-16(23)7-3-6-15(22)26-14-5-
InchiKey: PMFZTSVNEANZQA-UHFFFAOYSA-N
Formula: C17H12Cl3NO6
SMILES: O=C(CCCC(=O)Oc1c(Cl)cc(Cl)cc1Cl)Oc1ccccc1[N+](=O)[O-]
Mol. weight [g/mol]: 432.64

Physical Properties

Property code	Value	Unit	Source
gf	-189.52	kJ/mol	Joback Method
hf	-514.61	kJ/mol	Joback Method
hfus	55.84	kJ/mol	Joback Method
hvap	108.69	kJ/mol	Joback Method
log10ws	-6.87		Crippen Method
logp	5.236		Crippen Method
mcvol	271.890	ml/mol	McGowan Method
pc	1966.56	kPa	Joback Method
rinpol	3190.00		NIST Webbook
rinpol	3190.00		NIST Webbook
tb	1078.35	K	Joback Method
tc	1338.62	K	Joback Method
tf	761.96	K	Joback Method
vc	1.048	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	746.10	J/mol×K	1078.35	Joback Method
cpg	751.22	J/mol×K	1121.73	Joback Method
cpg	754.96	J/mol×K	1165.11	Joback Method
cpg	757.34	J/mol×K	1208.48	Joback Method
cpg	758.40	J/mol×K	1251.86	Joback Method
cpg	758.16	J/mol×K	1295.24	Joback Method
cpg	756.66	J/mol×K	1338.62	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=U393324&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