Glutaric acid, 3-chlorophenyl 2-nitrophenyl ester

Inchi: InChI=1S/C17H14ClNO6/c18-12-5-3-6-13(11-12)24-16(20)9-4-10-17(21)25-15-8-2-1-7-1
InchiKey: XBSSPKZELQSOHI-UHFFFAOYSA-N
Formula: C17H14ClNO6
SMILES: O=C(CCCC(=O)Oc1ccccc1[N+](=O)[O-])Oc1cccc(Cl)c1
Mol. weight [g/mol]: 363.75

Physical Properties

Property code	Value	Unit	Source
gf	-146.40	kJ/mol	Joback Method
hf	-460.19	kJ/mol	Joback Method
hfus	48.22	kJ/mol	Joback Method
hvap	98.60	kJ/mol	Joback Method
log10ws	-5.50		Crippen Method
logp	3.929		Crippen Method
mcvol	247.410	ml/mol	McGowan Method
pc	2161.32	kPa	Joback Method
rinpol	2902.00		NIST Webbook
rinpol	2902.00		NIST Webbook
tb	993.53	K	Joback Method
tc	1245.92	K	Joback Method
tf	677.08	K	Joback Method
vc	0.951	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	721.42	J/mol×K	993.53	Joback Method
cpg	729.72	J/mol×K	1035.59	Joback Method
cpg	736.68	J/mol×K	1077.66	Joback Method
cpg	742.35	J/mol×K	1119.72	Joback Method
cpg	746.76	J/mol×K	1161.79	Joback Method
cpg	749.95	J/mol×K	1203.85	Joback Method
cpg	751.97	J/mol×K	1245.92	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393321&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