Glutaric acid, 2,3-dichlorophenyl 2-nitrophenyl ester

Inchi: InChI=1S/C17H13Cl2NO6/c18-11-5-3-8-14(17(11)19)26-16(22)10-4-9-15(21)25-13-7-2-1

InchiKey: REOVEUZWALQAAY-UHFFFAOYSA-N

Formula: C17H13Cl2NO6

SMILES: O=C(CCCC(=O)Oc1cccc(Cl)c1Cl)Oc1ccccc1[N+](=O)[O-]

Mol. weight [g/mol]: 398.19

Physical Properties

Property code	Value	Unit	Source
gf	-167.96	kJ/mol	Joback Method
hf	-487.40	kJ/mol	Joback Method
hfus	52.03	kJ/mol	Joback Method
hvap	103.65	kJ/mol	Joback Method
log10ws	-6.19		Crippen Method
logp	4.583		Crippen Method
mcvol	259.650	ml/mol	McGowan Method
pc	2060.49	kPa	Joback Method
rinpol	3117.00		NIST Webbook
rinpol	3117.00		NIST Webbook
tb	1035.94	K	Joback Method
tc	1292.06	K	Joback Method
tf	719.52	K	Joback Method
vc	1.000	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	734.75	J/mol×K	1035.94	Joback Method
cpg	741.48	J/mol×K	1078.63	Joback Method
cpg	746.86	J/mol×K	1121.31	Joback Method
cpg	750.92	J/mol×K	1164.00	Joback Method
cpg	753.70	J/mol×K	1206.68	Joback Method
cpg	755.23	J/mol×K	1249.37	Joback Method
cpg	755.56	J/mol×K	1292.06	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393322&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