Glutaric acid, 2,2-dichloroethyl 2-nitrophenyl ester

Inchi: InChI=1S/C13H13Cl2NO6/c14-11(15)8-21-12(17)6-3-7-13(18)22-10-5-2-1-4-9(10)16(19)

InchiKey: JFDBLBYFBRQIQE-UHFFFAOYSA-N

Formula: C13H13Cl2NO6

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

Mol. weight [g/mol]: 350.15

Physical Properties

Property code	Value	Unit	Source
gf	-297.23	kJ/mol	Joback Method
hf	-623.71	kJ/mol	Joback Method
hfus	44.88	kJ/mol	Joback Method
hvap	90.75	kJ/mol	Joback Method
log10ws	-4.30		Crippen Method
logp	3.017		Crippen Method
mcvol	227.050	ml/mol	McGowan Method
pc	2241.88	kPa	Joback Method
rinpol	2527.00		NIST Webbook
rinpol	2527.00		NIST Webbook
tb	907.34	K	Joback Method
tc	1144.41	K	Joback Method
tf	607.98	K	Joback Method
vc	0.877	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	627.36	J/mol×K	907.34	Joback Method
cpg	636.40	J/mol×K	946.85	Joback Method
cpg	644.32	J/mol×K	986.36	Joback Method
cpg	651.14	J/mol×K	1025.88	Joback Method
cpg	656.88	J/mol×K	1065.39	Joback Method
cpg	661.57	J/mol×K	1104.90	Joback Method
cpg	665.22	J/mol×K	1144.41	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393316&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