Glutaric acid, ethyl 3-nitrophenyl ester

Inchi: InChI=1S/C13H15NO6/c1-2-19-12(15)7-4-8-13(16)20-11-6-3-5-10(9-11)14(17)18/h3,5-6,
InchiKey: WFZFKNUUUPOIHR-UHFFFAOYSA-N
Formula: C13H15NO6
SMILES: CCOC(=O)CCCC(=O)Oc1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]: 281.26

Physical Properties

Property code	Value	Unit	Source
gf	-270.93	kJ/mol	Joback Method
hf	-586.95	kJ/mol	Joback Method
hfus	40.01	kJ/mol	Joback Method
hvap	82.37	kJ/mol	Joback Method
log10ws	-3.39		Crippen Method
logp	2.234		Crippen Method
mcvol	202.570	ml/mol	McGowan Method
pc	2388.85	kPa	Joback Method
rinpol	2224.00		NIST Webbook
rinpol	2224.00		NIST Webbook
tb	832.92	K	Joback Method
tc	1060.93	K	Joback Method
tf	563.14	K	Joback Method
vc	0.785	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	587.32	J/mol×K	832.92	Joback Method
cpg	598.77	J/mol×K	870.92	Joback Method
cpg	609.15	J/mol×K	908.92	Joback Method
cpg	618.46	J/mol×K	946.92	Joback Method
cpg	626.72	J/mol×K	984.92	Joback Method
cpg	633.95	J/mol×K	1022.93	Joback Method
cpg	640.15	J/mol×K	1060.93	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U358886&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

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