Glutaric acid, di(2-(2-nitrophenyl)ethyl) ester

Inchi: InChI=1S/C21H22N2O8/c24-20(30-14-12-16-6-1-3-8-18(16)22(26)27)10-5-11-21(25)31-1
InchiKey: XCMCYKQLHRWBCJ-UHFFFAOYSA-N
Formula: C21H22N2O8
SMILES: O=C(CCCC(=O)OCCc1ccccc1[N+](=O)[O-])OCCc1ccccc1[N+](=O)[O-]
Mol. weight [g/mol]: 430.41

Physical Properties

Property code	Value	Unit	Source
gf	-65.24	kJ/mol	Joback Method
hf	-537.77	kJ/mol	Joback Method
hfus	65.75	kJ/mol	Joback Method
hvap	119.71	kJ/mol	Joback Method
log10ws	-5.85		Crippen Method
logp	3.545		Crippen Method
mcvol	308.950	ml/mol	McGowan Method
pc	1618.07	kPa	Joback Method
rinpol	3560.00		NIST Webbook
tb	1199.46	K	Joback Method
tc	1470.14	K	Joback Method
tf	835.85	K	Joback Method
vc	1.208	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1009.73	J/mol×K	1199.46	Joback Method
cpg	1014.72	J/mol×K	1244.57	Joback Method
cpg	1018.17	J/mol×K	1289.69	Joback Method
cpg	1020.17	J/mol×K	1334.80	Joback Method
cpg	1020.80	J/mol×K	1379.91	Joback Method
cpg	1020.14	J/mol×K	1425.03	Joback Method
cpg	1018.29	J/mol×K	1470.14	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377527&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