Glutaric acid, dodec-2-en-1-yl 4-nitrophenyl ester

Inchi: InChI=1S/C23H33NO6/c1-2-3-4-5-6-7-8-9-10-11-19-29-22(25)13-12-14-23(26)30-21-17-
InchiKey: BCEXNCFZVUCOCR-ZHACJKMWSA-N
Formula: C23H33NO6
SMILES: CCCCCCCCCC=CCOC(=O)CCCC(=O)Oc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 419.51

Physical Properties

Property code	Value	Unit	Source
gf	-106.51	kJ/mol	Joback Method
hf	-676.13	kJ/mol	Joback Method
hfus	66.11	kJ/mol	Joback Method
hvap	104.59	kJ/mol	Joback Method
log10ws	-7.43		Crippen Method
logp	5.911		Crippen Method
mcvol	339.170	ml/mol	McGowan Method
pc	1145.99	kPa	Joback Method
rinpol	3223.00		NIST Webbook
rinpol	3223.00		NIST Webbook
tb	1065.88	K	Joback Method
tc	1304.94	K	Joback Method
tf	670.76	K	Joback Method
vc	1.325	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1139.77	J/mol×K	1065.88	Joback Method
cpg	1152.82	J/mol×K	1105.72	Joback Method
cpg	1164.53	J/mol×K	1145.57	Joback Method
cpg	1174.98	J/mol×K	1185.41	Joback Method
cpg	1184.24	J/mol×K	1225.25	Joback Method
cpg	1192.39	J/mol×K	1265.10	Joback Method
cpg	1199.51	J/mol×K	1304.94	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391980&Units=SI

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