Glutaric acid, 3-nitro-4-methoxybenzyl undecyl ester

Inchi: InChI=1S/C24H37NO7/c1-3-4-5-6-7-8-9-10-11-17-31-23(26)13-12-14-24(27)32-19-20-15
InchiKey: ADIYGWSEOSEJAY-UHFFFAOYSA-N
Formula: C24H37NO7
SMILES: CCCCCCCCCCCOC(=O)CCCC(=O)OCc1ccc(OC)c([N+](=O)[O-])c1
Mol. weight [g/mol]: 451.55

Physical Properties

Property code	Value	Unit	Source
gf	-292.94	kJ/mol	Joback Method
hf	-957.68	kJ/mol	Joback Method
hfus	69.30	kJ/mol	Joback Method
hvap	109.93	kJ/mol	Joback Method
log10ws	-7.54		Crippen Method
logp	5.891		Crippen Method
mcvol	363.430	ml/mol	McGowan Method
pc	1018.13	kPa	Joback Method
rinpol	3459.00		NIST Webbook
tb	1112.00	K	Joback Method
tc	1365.23	K	Joback Method
tf	721.86	K	Joback Method
vc	1.419	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1252.91	J/mol×K	1112.00	Joback Method
cpg	1264.16	J/mol×K	1154.21	Joback Method
cpg	1273.33	J/mol×K	1196.41	Joback Method
cpg	1280.45	J/mol×K	1238.62	Joback Method
cpg	1285.57	J/mol×K	1280.82	Joback Method
cpg	1288.73	J/mol×K	1323.03	Joback Method
cpg	1289.97	J/mol×K	1365.23	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=U377049&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