Glutaric acid, 3-nitrophenethyl undecyl ester

Inchi: InChI=1S/C24H37NO6/c1-2-3-4-5-6-7-8-9-10-18-30-23(26)15-12-16-24(27)31-19-17-21-
InchiKey: NUUNDBWLJVNUOA-UHFFFAOYSA-N
Formula: C24H37NO6
SMILES: CCCCCCCCCCCOC(=O)CCCC(=O)OCCc1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]: 435.55

Physical Properties

Property code	Value	Unit	Source
gf	-178.31	kJ/mol	Joback Method
hf	-813.99	kJ/mol	Joback Method
hfus	68.50	kJ/mol	Joback Method
hvap	106.86	kJ/mol	Joback Method
log10ws	-7.35		Crippen Method
logp	5.925		Crippen Method
mcvol	357.560	ml/mol	McGowan Method
pc	1039.24	kPa	Joback Method
rinpol	3338.00		NIST Webbook
tb	1084.60	K	Joback Method
tc	1329.30	K	Joback Method
tf	687.11	K	Joback Method
vc	1.401	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1229.98	J/mol×K	1084.60	Joback Method
cpg	1243.08	J/mol×K	1125.38	Joback Method
cpg	1254.51	J/mol×K	1166.17	Joback Method
cpg	1264.34	J/mol×K	1206.95	Joback Method
cpg	1272.64	J/mol×K	1247.73	Joback Method
cpg	1279.48	J/mol×K	1288.52	Joback Method
cpg	1284.92	J/mol×K	1329.30	Joback Method

Sources

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=U376754&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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