Glutaric acid, 2-nitro-3-chlorobenzyl undecyl ester

Inchi: InChI=1S/C23H34ClNO6/c1-2-3-4-5-6-7-8-9-10-17-30-21(26)15-12-16-22(27)31-18-19-1

InchiKey: UCUKVNXSEYTTGC-UHFFFAOYSA-N

Formula: C23H34ClNO6

SMILES: CCCCCCCCCCCOC(=O)CCCC(=O)OCc1cccc(Cl)c1[N+](=O)[O-]

Mol. weight [g/mol]: 455.97

Physical Properties

Property code	Value	Unit	Source
gf	-208.29	kJ/mol	Joback Method
hf	-820.56	kJ/mol	Joback Method
hfus	69.72	kJ/mol	Joback Method
hvap	109.68	kJ/mol	Joback Method
log10ws	-8.11		Crippen Method
logp	6.536		Crippen Method
mcvol	355.710	ml/mol	McGowan Method
pc	1069.36	kPa	Joback Method
rinpol	3292.00		NIST Webbook
tb	1104.13	K	Joback Method
tc	1353.02	K	Joback Method
tf	718.28	K	Joback Method
vc	1.395	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1187.24	J/mol×K	1104.13	Joback Method
cpg	1198.65	J/mol×K	1145.61	Joback Method
cpg	1208.39	J/mol×K	1187.09	Joback Method
cpg	1216.52	J/mol×K	1228.57	Joback Method
cpg	1223.10	J/mol×K	1270.06	Joback Method
cpg	1228.19	J/mol×K	1311.54	Joback Method
cpg	1231.85	J/mol×K	1353.02	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=U377034&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