Glutaric acid, monoamide, N-(5-chloro-2-methoxyphenyl)-, undecyl ester

Inchi: InChI=1S/C23H36ClNO4/c1-3-4-5-6-7-8-9-10-11-17-29-23(27)14-12-13-22(26)25-20-18-

InchiKey: NBEVEAXUYAFWMG-UHFFFAOYSA-N

Formula: C23H36ClNO4

SMILES: CCCCCCCCCCCOC(=O)CCCC(O)=Nc1cc(Cl)ccc1OC

Mol. weight [g/mol]: 425.99

Physical Properties

Property code	Value	Unit	Source
hf	-777.02	kJ/mol	Joback Method
hvap	106.42	kJ/mol	Joback Method
log10ws	-7.39		Crippen Method
logp	7.181		Crippen Method
mcvol	348.270	ml/mol	McGowan Method
pc	1013.59	kPa	Joback Method
rinpol	3519.00		NIST Webbook
tb	1067.16	K	Joback Method
tc	1310.89	K	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=U360761&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

hf: Enthalpy of formation 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