Glutaric acid, monoamide, N-(4-chlorophenyl)-, dodecyl ester

Inchi: InChI=1S/C23H36ClNO3/c1-2-3-4-5-6-7-8-9-10-11-19-28-23(27)14-12-13-22(26)25-21-1

InchiKey: XHCSRQJMOXXDFA-UHFFFAOYSA-N

Formula: C23H36ClNO3

SMILES: CCCCCCCCCCCCOC(=O)CCCC(=O)Nc1ccc(Cl)cc1

Mol. weight [g/mol]: 409.99

Physical Properties

Property code	Value	Unit	Source
gf	-39.82	kJ/mol	Joback Method
hf	-612.64	kJ/mol	Joback Method
hfus	62.66	kJ/mol	Joback Method
hvap	96.45	kJ/mol	Joback Method
log10ws	-7.50		Crippen Method
logp	6.913		Crippen Method
mcvol	342.400	ml/mol	McGowan Method
pc	1092.82	kPa	Joback Method
rinpol	3463.00		NIST Webbook
tb	975.06	K	Joback Method
tc	1193.88	K	Joback Method
tf	592.58	K	Joback Method
vc	1.329	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1115.30	J/mol×K	975.06	Joback Method
cpg	1130.82	J/mol×K	1011.53	Joback Method
cpg	1145.08	J/mol×K	1048.00	Joback Method
cpg	1158.13	J/mol×K	1084.47	Joback Method
cpg	1170.04	J/mol×K	1120.94	Joback Method
cpg	1180.87	J/mol×K	1157.41	Joback Method
cpg	1190.67	J/mol×K	1193.88	Joback Method

Sources

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=U360791&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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