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

Inchi: InChI=1S/C19H28ClNO3/c1-2-3-4-5-6-7-15-24-19(23)10-8-9-18(22)21-17-13-11-16(20)1

InchiKey: VDHIQIJZGSGINQ-UHFFFAOYSA-N

Formula: C19H28ClNO3

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

Mol. weight [g/mol]: 353.88

Physical Properties

Property code	Value	Unit	Source
gf	-73.50	kJ/mol	Joback Method
hf	-530.08	kJ/mol	Joback Method
hfus	52.30	kJ/mol	Joback Method
hvap	87.55	kJ/mol	Joback Method
log10ws	-5.83		Crippen Method
logp	5.352		Crippen Method
mcvol	286.040	ml/mol	McGowan Method
pc	1433.72	kPa	Joback Method
rinpol	3058.00		NIST Webbook
tb	883.54	K	Joback Method
tc	1091.40	K	Joback Method
tf	547.50	K	Joback Method
vc	1.105	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	875.30	J/mol×K	883.54	Joback Method
cpg	889.75	J/mol×K	918.18	Joback Method
cpg	903.13	J/mol×K	952.83	Joback Method
cpg	915.47	J/mol×K	987.47	Joback Method
cpg	926.82	J/mol×K	1022.11	Joback Method
cpg	937.22	J/mol×K	1056.76	Joback Method
cpg	946.70	J/mol×K	1091.40	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360787&Units=SI
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

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