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

Inchi: InChI=1S/C16H22ClNO3/c1-2-3-4-12-21-16(20)7-5-6-15(19)18-14-10-8-13(17)9-11-14/h
InchiKey: XVJMDFLNNMXDIL-UHFFFAOYSA-N
Formula: C16H22ClNO3
SMILES: CCCCCOC(=O)CCCC(=O)Nc1ccc(Cl)cc1
Mol. weight [g/mol]: 311.80

Physical Properties

Property code	Value	Unit	Source
gf	-98.76	kJ/mol	Joback Method
hf	-468.16	kJ/mol	Joback Method
hfus	44.53	kJ/mol	Joback Method
hvap	80.87	kJ/mol	Joback Method
log10ws	-4.57		Crippen Method
logp	4.182		Crippen Method
mcvol	243.770	ml/mol	McGowan Method
pc	1806.16	kPa	Joback Method
rinpol	2736.00		NIST Webbook
tb	814.90	K	Joback Method
tc	1022.88	K	Joback Method
tf	513.69	K	Joback Method
vc	0.938	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	702.86	J/mol×K	814.90	Joback Method
cpg	716.54	J/mol×K	849.56	Joback Method
cpg	729.23	J/mol×K	884.23	Joback Method
cpg	740.98	J/mol×K	918.89	Joback Method
cpg	751.80	J/mol×K	953.55	Joback Method
cpg	761.74	J/mol×K	988.22	Joback Method
cpg	770.82	J/mol×K	1022.88	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360783&Units=SI

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