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

Inchi: InChI=1S/C18H26ClNO3/c1-2-3-4-5-6-14-23-18(22)9-7-8-17(21)20-16-12-10-15(19)11-1

InchiKey: XJDLVGOXMLACOR-UHFFFAOYSA-N

Formula: C18H26ClNO3

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

Mol. weight [g/mol]: 339.86

Physical Properties

Property code	Value	Unit	Source
gf	-81.92	kJ/mol	Joback Method
hf	-509.44	kJ/mol	Joback Method
hfus	49.71	kJ/mol	Joback Method
hvap	85.32	kJ/mol	Joback Method
log10ws	-5.41		Crippen Method
logp	4.962		Crippen Method
mcvol	271.950	ml/mol	McGowan Method
pc	1543.92	kPa	Joback Method
rinpol	2955.00		NIST Webbook
tb	860.66	K	Joback Method
tc	1067.86	K	Joback Method
tf	536.23	K	Joback Method
vc	1.050	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	817.00	J/mol×K	860.66	Joback Method
cpg	831.20	J/mol×K	895.19	Joback Method
cpg	844.37	J/mol×K	929.73	Joback Method
cpg	856.53	J/mol×K	964.26	Joback Method
cpg	867.72	J/mol×K	998.79	Joback Method
cpg	877.99	J/mol×K	1033.32	Joback Method
cpg	887.36	J/mol×K	1067.86	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=U360786&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