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

Inchi: InChI=1S/C17H24ClNO3/c1-2-3-4-5-13-22-17(21)8-6-7-16(20)19-15-11-9-14(18)10-12-1

InchiKey: YAYWMRISIBHCIC-UHFFFAOYSA-N

Formula: C17H24ClNO3

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

Mol. weight [g/mol]: 325.83

Physical Properties

Property code	Value	Unit	Source
gf	-90.34	kJ/mol	Joback Method
hf	-488.80	kJ/mol	Joback Method
hfus	47.12	kJ/mol	Joback Method
hvap	83.10	kJ/mol	Joback Method
log10ws	-4.99		Crippen Method
logp	4.572		Crippen Method
mcvol	257.860	ml/mol	McGowan Method
pc	1667.33	kPa	Joback Method
rinpol	2841.00		NIST Webbook
tb	837.78	K	Joback Method
tc	1045.03	K	Joback Method
tf	524.96	K	Joback Method
vc	0.994	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	759.50	J/mol×K	837.78	Joback Method
cpg	773.45	J/mol×K	872.32	Joback Method
cpg	786.39	J/mol×K	906.86	Joback Method
cpg	798.35	J/mol×K	941.41	Joback Method
cpg	809.37	J/mol×K	975.95	Joback Method
cpg	819.49	J/mol×K	1010.49	Joback Method
cpg	828.72	J/mol×K	1045.03	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360785&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

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