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

Inchi: InChI=1S/C13H16ClNO3/c1-2-18-13(17)5-3-4-12(16)15-11-8-6-10(14)7-9-11/h6-9H,2-5H

InchiKey: PWTZGDHOHVTTCK-UHFFFAOYSA-N

Formula: C13H16ClNO3

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

Mol. weight [g/mol]: 269.72

Physical Properties

Property code	Value	Unit	Source
gf	-124.02	kJ/mol	Joback Method
hf	-406.24	kJ/mol	Joback Method
hfus	36.76	kJ/mol	Joback Method
hvap	74.19	kJ/mol	Joback Method
log10ws	-3.31		Crippen Method
logp	3.012		Crippen Method
mcvol	201.500	ml/mol	McGowan Method
pc	2345.09	kPa	Joback Method
rinpol	2438.00		NIST Webbook
rinpol	2438.00		NIST Webbook
tb	746.26	K	Joback Method
tc	959.99	K	Joback Method
tf	479.88	K	Joback Method
vc	0.769	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	538.84	J/mol×K	746.26	Joback Method
cpg	551.48	J/mol×K	781.88	Joback Method
cpg	563.22	J/mol×K	817.50	Joback Method
cpg	574.09	J/mol×K	853.12	Joback Method
cpg	584.10	J/mol×K	888.74	Joback Method
cpg	593.28	J/mol×K	924.37	Joback Method
cpg	601.66	J/mol×K	959.99	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=U360780&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

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