3-Cyclopentylpropionic acid, 4-nitrophenyl ester

Inchi: InChI=1S/C14H17NO4/c16-14(10-5-11-3-1-2-4-11)19-13-8-6-12(7-9-13)15(17)18/h6-9,11

InchiKey: CFYBMLAAOGKARE-UHFFFAOYSA-N

Formula: C14H17NO4

SMILES: O=C(CCC1CCCC1)Oc1ccc([N+](=O)[O-])cc1

Mol. weight [g/mol]: 263.29

Physical Properties

Property code	Value	Unit	Source
gf	7.96	kJ/mol	Joback Method
hf	-302.31	kJ/mol	Joback Method
hfus	33.75	kJ/mol	Joback Method
hvap	75.70	kJ/mol	Joback Method
log10ws	-4.60		Crippen Method
logp	3.471		Crippen Method
mcvol	198.360	ml/mol	McGowan Method
pc	2480.12	kPa	Joback Method
rinpol	2132.00		NIST Webbook
rinpol	2132.00		NIST Webbook
tb	794.79	K	Joback Method
tc	1042.07	K	Joback Method
tf	513.15	K	Joback Method
vc	0.758	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	594.22	J/mol×K	794.79	Joback Method
cpg	609.41	J/mol×K	836.00	Joback Method
cpg	623.25	J/mol×K	877.22	Joback Method
cpg	635.80	J/mol×K	918.43	Joback Method
cpg	647.12	J/mol×K	959.64	Joback Method
cpg	657.28	J/mol×K	1000.86	Joback Method
cpg	666.34	J/mol×K	1042.07	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=U307136&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