Cyclopentanecarboxylic acid, 4-nitrophenyl ester

Inchi: InChI=1S/C12H13NO4/c14-12(9-3-1-2-4-9)17-11-7-5-10(6-8-11)13(15)16/h5-9H,1-4H2
InchiKey: PDWMECLUAQUZCV-UHFFFAOYSA-N
Formula: C12H13NO4
SMILES: O=C(Oc1ccc([N+](=O)[O-])cc1)C1CCCC1
Mol. weight [g/mol]: 235.24

Physical Properties

Property code	Value	Unit	Source
gf	-8.88	kJ/mol	Joback Method
hf	-261.03	kJ/mol	Joback Method
hfus	28.57	kJ/mol	Joback Method
hvap	71.25	kJ/mol	Joback Method
log10ws	-3.76		Crippen Method
logp	2.690		Crippen Method
mcvol	170.180	ml/mol	McGowan Method
pc	3032.27	kPa	Joback Method
rinpol	1904.00		NIST Webbook
rinpol	1904.00		NIST Webbook
tb	749.03	K	Joback Method
tc	1007.18	K	Joback Method
tf	490.61	K	Joback Method
vc	0.646	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	486.24	J/mol×K	749.03	Joback Method
cpg	500.92	J/mol×K	792.06	Joback Method
cpg	514.25	J/mol×K	835.08	Joback Method
cpg	526.29	J/mol×K	878.11	Joback Method
cpg	537.09	J/mol×K	921.13	Joback Method
cpg	546.73	J/mol×K	964.16	Joback Method
cpg	555.25	J/mol×K	1007.18	Joback Method

Sources

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=U307580&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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