Cyclohexanecarboxylic acid, 4-nitrophenyl ester

Inchi: InChI=1S/C13H15NO4/c15-13(10-4-2-1-3-5-10)18-12-8-6-11(7-9-12)14(16)17/h6-10H,1-

InchiKey: UCQFTYKBLBJWIO-UHFFFAOYSA-N

Formula: C13H15NO4

SMILES: O=C(Oc1ccc([N+](=O)[O-])cc1)C1CCCCC1

Mol. weight [g/mol]: 249.26

Physical Properties

Property code	Value	Unit	Source
gf	-12.56	kJ/mol	Joback Method
hf	-287.83	kJ/mol	Joback Method
hfus	29.06	kJ/mol	Joback Method
hvap	73.65	kJ/mol	Joback Method
log10ws	-4.18		Crippen Method
logp	3.080		Crippen Method
mcvol	184.270	ml/mol	McGowan Method
pc	2808.38	kPa	Joback Method
rinpol	2023.00		NIST Webbook
rinpol	2023.00		NIST Webbook
tb	776.18	K	Joback Method
tc	1036.29	K	Joback Method
tf	498.36	K	Joback Method
vc	0.695	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	542.68	J/mol×K	776.18	Joback Method
cpg	558.26	J/mol×K	819.53	Joback Method
cpg	572.31	J/mol×K	862.88	Joback Method
cpg	584.88	J/mol×K	906.24	Joback Method
cpg	596.03	J/mol×K	949.59	Joback Method
cpg	605.80	J/mol×K	992.94	Joback Method
cpg	614.26	J/mol×K	1036.29	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=U307708&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