

Nonoic acid, 4-nitrophenyl ester

Other names:	Nonoic acid, 4-nitrophenyl ester
Inchi:	InChI=1S/C15H21NO4/c1-2-3-4-5-6-7-8-15(17)20-14-11-9-13(10-12-14)16(18)19/h9-12H
InchiKey:	TZQXKOGMKYABTL-UHFFFAOYSA-N
Formula:	C15H21NO4
SMILES:	CCCCCCCCC(=O)Oc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]:	279.34

Physical Properties

Property code	Value	Unit	Source
hf	-438.17	kJ/mol	Cheméo Relay (1.0)
hfus	42.41	kJ/mol	Joback Method
hvap	96.48	kJ/mol	Cheméo Relay (1.0)
ie	9.12	eV	Cheméo Relay (1.0)
log10ws	-5.29		Cheméo Relay (1.0)
logp	4.251		Crippen Method
mcvol	223.310	ml/mol	McGowan Method
pc	1916.94	kPa	Joback Method
rinpol	2239.00		NIST Webbook
rinpol	2239.00		NIST Webbook
tb	603.22	K	Cheméo Relay (1.0)
tc	847.87	K	Cheméo Relay (1.0)
tf	333.90	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	660.01	J/mol×K	802.39	Joback Method
cpg	674.29	J/mol×K	838.85	Joback Method
cpg	687.53	J/mol×K	875.31	Joback Method
cpg	699.75	J/mol×K	911.78	Joback Method
cpg	711.01	J/mol×K	948.24	Joback Method
cpg	721.32	J/mol×K	984.70	Joback Method
cpg	730.73	J/mol×K	1021.16	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U358028&Units=SI

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

Latest version available from:

<https://www.chemeo.com/cid/20-518-4/Nonoic-acid-4-nitrophenyl-ester.pdf>

Generated by Cheméo on 2026-07-21 18:13:23.016738345 +0000 UTC m=+168698.858623758.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.