PENTANE, 1-NITRO-

Other names: 1-Nitropentane
Nitropentane
Inchi: InChI=1S/C5H11NO2/c1-2-3-4-5-6(7)8/h2-5H2,1H3
InchiKey: BVALZCVRLDMXOQ-UHFFFAOYSA-N
Formula: C5H11NO2
SMILES: CCCCC[N+](=O)[O-]
Mol. weight [g/mol]: 117.15

Physical Properties

Property code	Value	Unit	Source
af	0.4733		Cheméo Relay (1.0)
chl	-3324.00 ± 1.50	kJ/mol	NIST Webbook
gf	26.77	kJ/mol	Joback Method
hf	-172.56	kJ/mol	Cheméo Relay (1.0)
hfl	-215.00 ± 1.50	kJ/mol	NIST Webbook
hfus	20.07	kJ/mol	Joback Method
hvap	50.30 ± 0.20	kJ/mol	NIST Webbook
ie	10.58	eV	Cheméo Relay (1.0)
log10ws	-2.18		Cheméo Relay (1.0)
logp	1.453		Crippen Method
mcvol	98.730	ml/mol	McGowan Method
pc	3517.91	kPa	Joback Method
rinpol	896.00		NIST Webbook
rinpol	908.61		NIST Webbook
rinpol	947.00		NIST Webbook
rinpol	906.00		NIST Webbook
rinpol	865.90		NIST Webbook
rinpol	903.31		NIST Webbook
rinpol	910.36		NIST Webbook
rinpol	896.00		NIST Webbook
rinpol	941.00		NIST Webbook
rinpol	902.00		NIST Webbook
rinpol	946.04		NIST Webbook
rinpol	925.63		NIST Webbook
rinpol	941.00		NIST Webbook
rinpol	902.00		NIST Webbook
rinpol	910.36		NIST Webbook

rinpol	911.95		NIST Webbook
rinpol	913.83		NIST Webbook
rinpol	901.45		NIST Webbook
rinpol	902.40		NIST Webbook
rinpol	903.31		NIST Webbook
rinpol	904.49		NIST Webbook
rinpol	905.73		NIST Webbook
rinpol	907.12		NIST Webbook
rinpol	947.00		NIST Webbook
rinpol	865.90		NIST Webbook
rinpol	867.00		NIST Webbook
rinpol	869.00		NIST Webbook
rinpol	855.10		NIST Webbook
rinpol	890.00		NIST Webbook
rinpol	906.00		NIST Webbook
rinpol	905.00		NIST Webbook
ripol	1405.80		NIST Webbook
ripol	1414.00		NIST Webbook
ripol	1423.20		NIST Webbook
ripol	1418.80		NIST Webbook
ripol	1414.00		NIST Webbook
ripol	1409.60		NIST Webbook
ripol	1431.00		NIST Webbook
ripol	1434.50		NIST Webbook
ripol	1428.60		NIST Webbook
ripol	1428.60		NIST Webbook
tb	445.70	K	NIST Webbook
tc	642.86	K	Cheméo Relay (1.0)
tf	211.94	K	Cheméo Relay (1.0)
vc	0.361	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	209.12	J/mol×K	465.64	Joback Method
cpg	219.70	J/mol×K	499.71	Joback Method
cpg	229.76	J/mol×K	533.78	Joback Method
cpg	239.31	J/mol×K	567.84	Joback Method
cpg	248.37	J/mol×K	601.91	Joback Method
cpg	256.96	J/mol×K	635.98	Joback Method
cpg	265.10	J/mol×K	670.05	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	348.70	K	3.10	NIST Webbook

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C628057&Units=SI

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

Legend

af: Acentric Factor
chl: Standard liquid enthalpy of combustion
cpg: Ideal gas heat capacity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfl: Liquid phase 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
rinpol: Non-polar retention indices
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tbrp: Boiling point at reduced pressure

tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume