1-NITRODODECANE

Other names: Dodecane, 1-nitro-
Inchi: InChI=1S/C12H25NO2/c1-2-3-4-5-6-7-8-9-10-11-12-13(14)15/h2-12H2,1H3
InchiKey: MQEMKUTWMALMCC-UHFFFAOYSA-N
Formula: C12H25NO2
SMILES: CCCCCCCCCCCC[N+](=O)[O-]
Mol. weight [g/mol]: 215.34
CAS: 16891-99-9

Physical Properties

Property code	Value	Unit	Source
af	0.7572		Cheméo Relay (1.0)
gf	85.71	kJ/mol	Joback Method
hf	-346.66	kJ/mol	Cheméo Relay (1.0)
hfus	38.20	kJ/mol	Joback Method
hvap	81.75	kJ/mol	Cheméo Relay (1.0)
ie	10.22	eV	Cheméo Relay (1.0)
log10ws	-5.59		Cheméo Relay (1.0)
logp	4.184		Crippen Method
mcvol	197.360	ml/mol	McGowan Method
pc	1798.51	kPa	Joback Method
tb	550.36	K	Cheméo Relay (1.0)
tc	753.13	K	Cheméo Relay (1.0)
tf	281.13	K	Cheméo Relay (1.0)
vc	0.754	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	535.52	J/mol×K	625.80	Joback Method
cpg	551.82	J/mol×K	656.99	Joback Method
cpg	567.33	J/mol×K	688.18	Joback Method
cpg	582.06	J/mol×K	719.37	Joback Method
cpg	596.06	J/mol×K	750.56	Joback Method
cpg	609.34	J/mol×K	781.75	Joback Method

cpg	621.94	J/mol×K	812.93	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.45334e+01
Coeff. B	-4.75054e+03
Coeff. C	-9.96520e+01
Temperature range (K), min.	433.12
Temperature range (K), max.	614.78

Sources

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):

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C16891999&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

af: Acentric Factor

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

ie: Ionization energy

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume