Heptane, 1-nitro-

Other names: 1-Nitroheptane
Inchi: InChI=1S/C7H15NO2/c1-2-3-4-5-6-7-8(9)10/h2-7H2,1H3
InchiKey: UZONFOPDCXAZND-UHFFFAOYSA-N
Formula: C7H15NO2
SMILES: CCCCCCC[N+](=O)[O-]
Mol. weight [g/mol]: 145.20
CAS: 693-39-0

Physical Properties

Property code	Value	Unit	Source
gf	43.61	kJ/mol	Joback Method
hf	-198.57	kJ/mol	Joback Method
hfus	25.25	kJ/mol	Joback Method
hvap	47.77	kJ/mol	Joback Method
log10ws	-2.84		Crippen Method
logp	2.233		Crippen Method
mcvol	126.910	ml/mol	McGowan Method
pc	2835.36	kPa	Joback Method
rinpol	1150.00		NIST Webbook
tb	511.40	K	Joback Method
tc	710.38	K	Joback Method
tf	312.26	K	Joback Method
vc	0.509	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	293.28	J/mol×K	511.40	Joback Method
cpg	306.06	J/mol×K	544.56	Joback Method
cpg	318.21	J/mol×K	577.73	Joback Method
cpg	329.75	J/mol×K	610.89	Joback Method
cpg	340.71	J/mol×K	644.05	Joback Method
cpg	351.10	J/mol×K	677.21	Joback Method
cpg	360.94	J/mol×K	710.38	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.49366e+01
Coeff. B	-4.24265e+03
Coeff. C	-7.63000e+01
Temperature range (K), min.	365.92
Temperature range (K), max.	517.09

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C693390&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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

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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature

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