3,3-DIMETHYLPIPERIDINE

Other names: Piperidine, 3,3-dimethyl-
Inchi: InChI=1S/C7H15N/c1-7(2)4-3-5-8-6-7/h8H,3-6H2,1-2H3
InchiKey: CDODDZJCEADUQQ-UHFFFAOYSA-N
Formula: C7H15N
SMILES: CC1(C)CCCNC1
Mol. weight [g/mol]: 113.20
CAS: 1193-12-0

Physical Properties

Property code	Value	Unit	Source
af	0.3109		Cheméo Relay (1.0)
gf	114.73	kJ/mol	Joback Method
hf	-118.62	kJ/mol	Cheméo Relay (1.0)
hfus	9.01	kJ/mol	Joback Method
hvap	45.84	kJ/mol	Cheméo Relay (1.0)
ie	8.05 ± 0.05	eV	NIST Webbook
logp	1.396		Crippen Method
mcvol	108.610	ml/mol	McGowan Method
pc	3834.03	kPa	Joback Method
rinpol	870.00		NIST Webbook
tb	410.20	K	NIST Webbook
tc	599.62	K	Cheméo Relay (1.0)
tf	263.81	K	Cheméo Relay (1.0)
vc	0.372	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	216.01	J/mol×K	427.90	Joback Method
cpg	233.15	J/mol×K	464.78	Joback Method
cpg	249.12	J/mol×K	501.67	Joback Method
cpg	264.03	J/mol×K	538.55	Joback Method
cpg	278.00	J/mol×K	575.43	Joback Method
cpg	291.12	J/mol×K	612.32	Joback Method

cpg	303.49	J/mol×K	649.20	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.43187e+01
Coeff. B	-3.44392e+03
Coeff. C	-5.51720e+01
Temperature range (K), min.	300.62
Temperature range (K), max.	437.52

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=C1193120&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

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