2,2-DIMETHYL-1,3-PROPANEDIAMINE

Other names: 1,3-Propanediamine, 2,2-dimethyl-
2,2-Dimethyltrimethylenediamine
2,2-dimethylpropane-1,3-diamine
Neopentylenediamine
Inchi: InChI=1S/C5H14N2/c1-5(2,3-6)4-7/h3-4,6-7H2,1-2H3
InchiKey: DDHUNHGZUHZNKB-UHFFFAOYSA-N
Formula: C5H14N2
SMILES: CC(C)(CN)CN
Mol. weight [g/mol]: 102.18
CAS: 7328-91-8

Physical Properties

Property code	Value	Unit	Source
af	0.4520		Cheméo Relay (1.0)
gf	126.96	kJ/mol	Joback Method
hf	-115.42	kJ/mol	Cheméo Relay (1.0)
hfus	11.69	kJ/mol	Joback Method
hvap	49.65	kJ/mol	Cheméo Relay (1.0)
ie	8.45	eV	Cheméo Relay (1.0)
log10ws	-0.84		Cheméo Relay (1.0)
logp	-0.070		Crippen Method
mcvol	101.270	ml/mol	McGowan Method
pc	4082.92	kPa	Joback Method
tb	426.20	K	NIST Webbook
tc	611.58	K	Cheméo Relay (1.0)
tf	297.56	K	Cheméo Relay (1.0)
vc	0.339	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	226.99	J/mol×K	455.63	Joback Method
cpg	238.95	J/mol×K	490.33	Joback Method
cpg	250.18	J/mol×K	525.04	Joback Method

cpg	260.74	J/mol×K	559.74	Joback Method
cpg	270.65	J/mol×K	594.45	Joback Method
cpg	279.96	J/mol×K	629.15	Joback Method
cpg	288.68	J/mol×K	663.85	Joback Method
hfust	1.70	kJ/mol	301.70	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.56590e+01
Coeff. B	-4.04730e+03
Coeff. C	-5.96200e+01
Temperature range (K), min.	303.15
Temperature range (K), max.	450.76

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):

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=C7328918&Units=SI

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

hfust:	Enthalpy of fusion at a given temperature
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