

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
gf	126.96	kJ/mol	Joback Method
hf	-87.70	kJ/mol	Joback Method
hfus	11.69	kJ/mol	Joback Method
hvap	46.71	kJ/mol	Joback Method
log10ws	-0.54		Crippen Method
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	663.85	K	Joback Method
tf	315.05	K	Joback Method
vc	0.362	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	279.96	J/mol×K	629.15	Joback Method
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	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	$\ln(P_{vp}) = A + B/(T + C)$
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

The Yaws Handbook of Vapor Pressure: Crippen Method:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	https://en.wikipedia.org/wiki/Joback_method
NIST Webbook:	http://link.springer.com/article/10.1007/BF02311772
	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7328918&Units=SI

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
hfust:	Enthalpy of fusion at a given temperature
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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