

N,N,N'-Trimethyl-1,3-propanediamine

Other names:	1,3-Propanediamine, N,N,N'-trimethyl- 3-Dimethylamino-N-methylpropylamine N,N,N'-trimethylpropane-1,3-diamine
Inchi:	InChI=1S/C6H16N2/c1-7-5-4-6-8(2)3/h7H,4-6H2,1-3H3
InchiKey:	SORARJZLMNRBAQ-UHFFFAOYSA-N
Formula:	C6H16N2
SMILES:	CNCCCN(C)C
Mol. weight [g/mol]:	116.20
CAS:	4543-96-8

Physical Properties

Property code	Value	Unit	Source
gf	199.81	kJ/mol	Joback Method
hf	-46.17	kJ/mol	Joback Method
hfus	19.42	kJ/mol	Joback Method
hvap	37.43	kJ/mol	Joback Method
log10ws	-0.09		Crippen Method
logp	0.158		Crippen Method
mcvol	115.360	ml/mol	McGowan Method
pc	3145.56	kPa	Joback Method
tb	414.20	K	NIST Webbook
tc	567.84	K	Joback Method
tf	242.51	K	Joback Method
vc	0.424	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	227.50	J/mol×K	399.29	Joback Method
cpg	240.03	J/mol×K	427.38	Joback Method
cpg	252.05	J/mol×K	455.47	Joback Method
cpg	263.56	J/mol×K	483.57	Joback Method
cpg	274.60	J/mol×K	511.66	Joback Method
cpg	285.16	J/mol×K	539.75	Joback Method

cpg	295.26	J/mol×K	567.84	Joback Method
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Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.56528e+01
Coeff. B	-3.94941e+03
Coeff. C	-5.62840e+01
Temperature range (K), min.	313.32
Temperature range (K), max.	438.19

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/ci990307I
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=C4543968&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
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccol:	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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