N,N,2,2-Tetramethyl-1,3-propanediamine

Other names: 1,3-Propanediamine, N,N,2,2-tetramethyl-
N,N,2,2-tetramethylpropane-1,3-diamine
Inchi: InChI=1S/C7H18N2/c1-7(2,5-8)6-9(3)4/h5-6,8H2,1-4H3
InchiKey: ULDIVZQLPBUHAG-UHFFFAOYSA-N
Formula: C7H18N2
SMILES: CN(C)CC(C)(C)CN
Mol. weight [g/mol]: 130.23
CAS: 53369-71-4

Physical Properties

Property code	Value	Unit	Source
gf	188.13	kJ/mol	Joback Method
hf	-95.24	kJ/mol	Joback Method
hfus	14.69	kJ/mol	Joback Method
hvap	42.56	kJ/mol	Joback Method
log10ws	-0.52		Crippen Method
logp	0.533		Crippen Method
mcvol	129.450	ml/mol	McGowan Method
pc	3032.27	kPa	Joback Method
tb	429.70	K	NIST Webbook
tc	629.59	K	Joback Method
tf	286.80	K	Joback Method
vc	0.464	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	283.71	J/mol×K	441.30	Joback Method
cpg	298.62	J/mol×K	472.68	Joback Method
cpg	312.72	J/mol×K	504.06	Joback Method
cpg	326.05	J/mol×K	535.44	Joback Method
cpg	338.63	J/mol×K	566.83	Joback Method
cpg	350.51	J/mol×K	598.21	Joback Method
cpg	361.72	J/mol×K	629.59	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.56608e+01
Coeff. B	-4.07585e+03
Coeff. C	-6.05930e+01
Temperature range (K), min.	302.05
Temperature range (K), max.	454.42

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C53369714&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume