Homopiperazine

Other names:	1,4-Diazacycloheptane
	1H-1,4-Diazepine, hexahydro-
	Hexahydro-1,4-diazepine
	Trimethyleneethylenediamine
	perhydro-1,4-diazepine
Inchi:	InChI=1S/C5H12N2/c1-2-6-4-5-7-3-1/h6-7H,1-5H2
InchiKey:	FQUYSHZXSKYCSY-UHFFFAOYSA-N
Formula:	C5H12N2
SMILES:	C1CNCCNC1
Mol. weight [g/mol]:	100.16
CAS:	505-66-8

Physical Properties

Property code	Value	Unit	Source
gf	186.70	kJ/mol	Joback Method
hf	-2.41	kJ/mol	Joback Method
hfus	16.55	kJ/mol	Joback Method
hvap	41.15	kJ/mol	Joback Method
log10ws	-0.19		Crippen Method
logp	-0.431		Crippen Method
mcvol	90.410	ml/mol	McGowan Method
pc	5213.15	kPa	Joback Method
ripol	1525.00		NIST Webbook
tb	442.20	K	NIST Webbook
tb	442.25	K	NIST Webbook
tc	674.36	K	Joback Method
tf	364.27	K	Joback Method
vc	0.316	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	172.49	J/mol×K	439.39	Joback Method
cpg	187.60	J/mol×K	478.55	Joback Method

cpg	201.99	J/mol×K	517.71	Joback Method
cpg	215.68	J/mol×K	556.88	Joback Method
cpg	228.65	J/mol×K	596.04	Joback Method
cpg	240.91	J/mol×K	635.20	Joback Method
cpg	252.44	J/mol×K	674.36	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.55625e+01
Coeff. B	-4.13804e+03
Coeff. C	-6.40950e+01
Temperature range (K), min.	314.65
Temperature range (K), max.	467.77

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C505668&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

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:
https://www.chemeo.com/cid/63-327-9/Homopiperazine.pdf
Generated by Cheméo on 2024-04-25 08:52:01.171228228 +0000 UTC m=+16324370.091805539.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.