Neopentylamine

Other names:	1-Propanamine, 2,2-dimethyl-
	2,2-Dimethyl-1-propylamine
	2,2-Dimethylpropylamine
	neo-C5H11NH2
Inchi:	InChI=1S/C5H13N/c1-5(2,3)4-6/h4,6H2,1-3H3
InchiKey:	XDIAMRVROCPPBK-UHFFFAOYSA-N
Formula:	C5H13N
SMILES:	CC(C)(C)CN
Mol. weight [g/mol]:	87.16
CAS:	5813-64-9

Physical Properties

Property code	Value	Unit	Source
affp	928.30	kJ/mol	NIST Webbook
basg	894.00	kJ/mol	NIST Webbook
gf	60.51	kJ/mol	Joback Method
hf	-121.49	kJ/mol	Joback Method
hfus	6.49	kJ/mol	Joback Method
hvap	36.07	kJ/mol	Joback Method
ie	8.50	eV	NIST Webbook
ie	8.50 ± 0.10	eV	NIST Webbook
ie	9.30	eV	NIST Webbook
log10ws	-1.11		Crippen Method
logp	0.991		Crippen Method
mcvol	91.290	ml/mol	McGowan Method
pc	3801.00	kPa	Joback Method
tb	355.65 ± 5.00	K	NIST Webbook
tc	576.55	K	Joback Method
tf	231.79	K	Joback Method
vc	0.334	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	175.09	J/mol×K	383.10	Joback Method
cpg	186.67	J/mol×K	415.34	Joback Method
cpg	197.63	J/mol×K	447.58	Joback Method
cpg	208.00	J/mol×K	479.82	Joback Method
cpg	217.79	J/mol×K	512.07	Joback Method
cpg	227.04	J/mol×K	544.31	Joback Method
cpg	235.77	J/mol×K	576.55	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.32972e+01
Coeff. B	-2.38798e+03
Coeff. C	-8.05000e+01
Temperature range (K), min.	264.06
Temperature range (K), max.	379.53

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5813649&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

affp: Proton affinity

basg: Gas basicity

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
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