2-Propaneamine, N,N-diethyl-

Other names: (i-C3H7)N(C2H5)2
2-Propanamine, N,N-diethyl-
Diethylisopropylamine
Inchi: InChI=1S/C7H17N/c1-5-8(6-2)7(3)4/h7H,5-6H2,1-4H3
InchiKey: ULWOJODHECIZAU-UHFFFAOYSA-N
Formula: C7H17N
SMILES: CCN(CC)C(C)C
Mol. weight [g/mol]: 115.22
CAS: 6006-15-1

Physical Properties

Property code	Value	Unit	Source
affp	996.40	kJ/mol	NIST Webbook
basg	965.60	kJ/mol	NIST Webbook
gf	116.40	kJ/mol	Joback Method
hf	-125.56	kJ/mol	Joback Method
hfus	13.38	kJ/mol	Joback Method
hvap	32.83	kJ/mol	Joback Method
log10ws	-1.43		Crippen Method
logp	1.737		Crippen Method
mcvol	119.470	ml/mol	McGowan Method
pc	2817.33	kPa	Joback Method
rinpol	742.00		NIST Webbook
rinpol	737.00		NIST Webbook
tb	381.65 ± 3.00	K	NIST Webbook
tc	537.88	K	Joback Method
tf	186.12	K	Joback Method
vc	0.440	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	221.23	J/mol×K	371.56	Joback Method
cpg	234.61	J/mol×K	399.28	Joback Method

cpg	247.47	J/mol×K	427.00	Joback Method
cpg	259.82	J/mol×K	454.72	Joback Method
cpg	271.66	J/mol×K	482.44	Joback Method
cpg	283.03	J/mol×K	510.16	Joback Method
cpg	293.92	J/mol×K	537.88	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.56401e+01
Coeff. B	-3.68570e+03
Coeff. C	-4.72490e+01
Temperature range (K), min.	287.32
Temperature range (K), max.	404.09

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6006151&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

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

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume