2-(Propylamino)ethanol

Other names: Ethanol, 2-(propylamino)-
Inchi: InChI=1S/C5H13NO/c1-2-3-6-4-5-7/h6-7H,2-5H2,1H3
InchiKey: BCLSJHWBDUYDTR-UHFFFAOYSA-N
Formula: C5H13NO
SMILES: CCCNCCO
Mol. weight [g/mol]: 103.16
CAS: 16369-21-4

Physical Properties

Property code	Value	Unit	Source
gf	-56.21	kJ/mol	Joback Method
hf	-245.29	kJ/mol	Joback Method
hfus	17.89	kJ/mol	Joback Method
hvap	49.84	kJ/mol	Joback Method
log10ws	-0.37		Crippen Method
logp	-0.022		Crippen Method
mcvol	97.160	ml/mol	McGowan Method
pc	3940.66	kPa	Joback Method
tb	456.15	K	Joback Method
tc	622.16	K	Joback Method
tf	259.59	K	Joback Method
vc	0.369	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	209.54	J/mol×K	456.15	Joback Method
cpg	218.58	J/mol×K	483.82	Joback Method
cpg	227.28	J/mol×K	511.49	Joback Method
cpg	235.64	J/mol×K	539.16	Joback Method
cpg	243.66	J/mol×K	566.82	Joback Method
cpg	251.37	J/mol×K	594.49	Joback Method
cpg	258.76	J/mol×K	622.16	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	455.20	K	99.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.49950e+01
Coeff. B	-4.13921e+03
Coeff. C	-6.76820e+01
Temperature range (K), min.	349.12
Temperature range (K), max.	495.13

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16369214&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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume