2-Propanol, 1-(diethylamino)-

Other names: 1-Diethylamino-2-propanol
1-diethylaminopropan-2-ol
Inchi: InChI=1S/C7H17NO/c1-4-8(5-2)6-7(3)9/h7,9H,4-6H2,1-3H3
InchiKey: BHUXAQIVYLDUQV-UHFFFAOYSA-N
Formula: C7H17NO
SMILES: CCN(CC)CC(C)O
Mol. weight [g/mol]: 131.22
CAS: 4402-32-8

Physical Properties

Property code	Value	Unit	Source
gf	-20.42	kJ/mol	Joback Method
hf	-277.79	kJ/mol	Joback Method
hfus	17.47	kJ/mol	Joback Method
hvap	49.51	kJ/mol	Joback Method
log10ws	-0.70		Crippen Method
logp	0.709		Crippen Method
mcvol	125.340	ml/mol	McGowan Method
pc	3114.04	kPa	Joback Method
tb	463.74	K	Joback Method
tc	626.19	K	Joback Method
tf	246.94	K	Joback Method
vc	0.459	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	279.21	J/mol×K	463.74	Joback Method
cpg	290.95	J/mol×K	490.81	Joback Method
cpg	302.21	J/mol×K	517.89	Joback Method
cpg	313.00	J/mol×K	544.96	Joback Method
cpg	323.33	J/mol×K	572.04	Joback Method
cpg	333.23	J/mol×K	599.11	Joback Method
cpg	342.70	J/mol×K	626.19	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	330.20	K	1.70	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.17670e+01
Coeff. B	-3.20978e+03
Coeff. C	-6.67090e+01
Temperature range (K), min.	346.32
Temperature range (K), max.	563.92

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4402328&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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume