Diisopropanolamine

Other names:	1,1'-Iminobis[2-propanol]
	1,1'-Iminodi-2-propanol
	1,1'-iminodipropan-2-ol
	2-Propanol, 1,1'-iminobis-
	2-Propanol, 1,1'-iminodi-
	BIS(2-PROPANOL)AMINE
	Bis(2-hydroxypropyl)amine
	DIPA
	DIPA (alcohol)
	DIPROPYL-2,2'-DIHYDROXY-AMINE
	Di(2-hydroxy-n-propyl) amine
	Di-2-propanolamine
	N,N-Bis(2-hydroxypropyl)amine
	NSC 4963
Inchi:	InChI=1S/C6H15NO2/c1-5(8)3-7-4-6(2)9/h5-9H,3-4H2,1-2H3
InchiKey:	LVTYICIALWPMFW-UHFFFAOYSA-N
Formula:	C6H15NO2
SMILES:	CC(O)CNCC(C)O
Mol. weight [g/mol]:	133.19
CAS:	110-97-4

Physical Properties

Property code	Value	Unit	Source
gf	-189.49	kJ/mol	Joback Method
hf	-428.72	kJ/mol	Joback Method
hfus	17.53	kJ/mol	Joback Method
hvap	67.97	kJ/mol	Joback Method
log10ws	-0.27		Crippen Method
logp	-0.662		Crippen Method
mcvol	117.120	ml/mol	McGowan Method
pc	4000.70	kPa	Joback Method
tb	521.85	K	NIST Webbook
tc	736.51	K	Joback Method
tf	315.15	K	NIST Webbook
vc	0.432	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	300.16	J/mol×K	570.33	Joback Method
cpg	309.37	J/mol×K	598.03	Joback Method
cpg	318.18	J/mol×K	625.72	Joback Method
cpg	326.61	J/mol×K	653.42	Joback Method
cpg	334.66	J/mol×K	681.12	Joback Method
cpg	342.35	J/mol×K	708.81	Joback Method
cpg	349.69	J/mol×K	736.51	Joback Method
hvapt	68.00	kJ/mol	455.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	522.70	K	99.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.83698e+01
Coeff. B	-5.99031e+03
Coeff. C	-8.62380e+01
Temperature range (K), min.	417.52
Temperature range (K), max.	544.97

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	2.16928e+02
Coeff. B	-2.04874e+04
Coeff. C	-2.81228e+01

Coeff. D	1.06841e-05
Temperature range (K), min.	318.15
Temperature range (K), max.	672.00

Sources

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
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1327
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C110974&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1327

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
hvapt:	Enthalpy of vaporization at a given temperature
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