

(Diisopropylamino)ethanol

Other names:	2-(Diisopropylamino)ethanol 2-(Diisopropylamino)ethyl alcohol Diisopropylethanolamine Ethanol, 2-(diisopropylamino)- Ethanol, 2-[bis(1-methylethyl)amino]- Ethanol, diisopropylamino- N,N-Diisopropylaminoethanol N,N-Diisopropylethanolamine NSC 45475 UN 2825
Inchi:	InChI=1S/C8H19NO/c1-7(2)9(5-6-10)8(3)4/h7-8,10H,5-6H2,1-4H3
InchiKey:	ZYWUVGFIXPNBDL-UHFFFAOYSA-N
Formula:	C8H19NO
SMILES:	CC(C)N(CCO)C(C)C
Mol. weight [g/mol]:	145.24
CAS:	96-80-0

Physical Properties

Property code	Value	Unit	Source
gf	-14.44	kJ/mol	Joback Method
hf	-303.71	kJ/mol	Joback Method
hfus	16.54	kJ/mol	Joback Method
hvap	51.35	kJ/mol	Joback Method
log10ws	-1.23		Crippen Method
logp	1.098		Crippen Method
mcvol	139.430	ml/mol	McGowan Method
pc	2829.33	kPa	Joback Method
tb	463.20	K	NIST Webbook
tc	650.98	K	Joback Method
tf	233.90 ± 0.60	K	NIST Webbook
vc	0.508	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	323.15	J/mol×K	486.18	Joback Method
cpg	336.07	J/mol×K	513.65	Joback Method
cpg	348.45	J/mol×K	541.11	Joback Method
cpg	360.30	J/mol×K	568.58	Joback Method
cpg	371.64	J/mol×K	596.05	Joback Method
cpg	382.49	J/mol×K	623.51	Joback Method
cpg	392.86	J/mol×K	650.98	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.61053e+01
Coeff. B	-4.51777e+03
Coeff. C	-6.99060e+01
Temperature range (K), min.	355.52
Temperature range (K), max.	488.46

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C96800&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

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

h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log10 of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
p_c:	Critical Pressure
p_{vap}:	Vapor pressure
t_b:	Normal Boiling Point Temperature
t_c:	Critical Temperature
t_f:	Normal melting (fusion) point
v_c:	Critical Volume

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