2-(DIBUTYLAMINO)ETHANOL

Other names:	(Dibutylamino)ethanol
	2-(Dibutylamino)ethanol
	2-Ethamolamine, N,N-dibutyl-
	2-N-Dibutylaminoethanol
	2-di-n-Butylaminoethanol
	BU2AE
	DBAE
	Di(n-butyl)ethanolamine
	Dibutylethanolamine
	N,N-(Dibutylamino)ethanol
	N,N-Dibutyl-2-hydroxyethylamine
	N,N-Dibutyl-N-(2-hydroxyethyl)amine
	N,N-Dibutylethanolamine
	N,N-di-n-Butylaminoethanol
	N,N-di-n-Butylethanolamine
	NSC 6330
	UN 2873
	«beta»-N-Dibutylaminoethyl alcohol
Inchi:	InChI=1S/C10H23NO/c1-3-5-7-11(9-10-12)8-6-4-2/h12H,3-10H2,1-2H3
InchiKey:	IWSZDQRGNFLMJS-UHFFFAOYSA-N
Formula:	C10H23NO
SMILES:	CCCCN(CCO)CCCC
Mol. weight [g/mol]:	173.30

Physical Properties

Property code	Value	Unit	Source
af	0.7441		Cheméo Relay (1.0)
gf	7.28	kJ/mol	Joback Method
hf	-358.75	kJ/mol	Cheméo Relay (1.0)
hfus	28.76	kJ/mol	Joback Method
hvap	71.54	kJ/mol	Cheméo Relay (1.0)
ie	8.02	eV	Cheméo Relay (1.0)
log10ws	-0.98		Cheméo Relay (1.0)
logp	1.881		Crippen Method
mcvol	167.610	ml/mol	McGowan Method
pc	2293.71	kPa	Joback Method
tb	502.70	K	NIST Webbook

tc	678.57	K	Cheméo Relay (1.0)
tf	225.47	K	Cheméo Relay (1.0)
vc	0.606	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	415.92	J/mol×K	532.82	Joback Method
cpg	429.74	J/mol×K	559.07	Joback Method
cpg	443.00	J/mol×K	585.33	Joback Method
cpg	455.72	J/mol×K	611.58	Joback Method
cpg	467.91	J/mol×K	637.83	Joback Method
cpg	479.61	J/mol×K	664.09	Joback Method
cpg	490.81	J/mol×K	690.34	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C102818&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

af: Acentric Factor
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
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume