

Ethanol, 2-(butylamino)-

Other names: 2-(N-Monobutylamino)ethanol
2-(butylamino)ethanol
2-(n-Butylamino)ethanol
2-Butylaminoethanol
Butyl(2-hydroxyethyl)amine
Butylethanolamine
Butylmonoethanolamine
N-Butyl monoethanolamine
N-butylethanolamine
N-n-Butylethanolamine
NSC 1098
n-Butylaminoethanol

Inchi: InChI=1S/C6H15NO/c1-2-3-4-7-5-6-8/h7-8H,2-6H2,1H3

InchiKey: LJDSTRZHPWMDPG-UHFFFAOYSA-N

Formula: C6H15NO

SMILES: CCCCNCCO

Mol. weight [g/mol]: 117.19

CAS: 111-75-1

Physical Properties

Property code	Value	Unit	Source
gf	-47.79	kJ/mol	Joback Method
hf	-265.93	kJ/mol	Joback Method
hfus	20.48	kJ/mol	Joback Method
hvap	52.06	kJ/mol	Joback Method
log10ws	-0.79		Crippen Method
logp	0.368		Crippen Method
mcvol	111.250	ml/mol	McGowan Method
pc	3505.43	kPa	Joback Method
tb	479.03	K	Joback Method
tc	644.08	K	Joback Method
tf	270.86	K	Joback Method
vc	0.425	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	250.46	J/mol×K	479.03	Joback Method
cpg	260.55	J/mol×K	506.54	Joback Method
cpg	270.24	J/mol×K	534.05	Joback Method
cpg	279.55	J/mol×K	561.55	Joback Method
cpg	288.49	J/mol×K	589.06	Joback Method
cpg	297.06	J/mol×K	616.57	Joback Method
cpg	305.28	J/mol×K	644.08	Joback Method

Sources

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Solubility of Carbon Dioxide in Aqueous Solutions of Three Secondary Amines *Met(Boc₂)₂(Boc₂)-laminino)ethanol, 2-(Isopropylamino)ethanol, and 2-(Ethylamino)ethanol Secondary Alkanolamine Solutions:*

<https://www.doi.org/10.1021/acs.jced.7b00364>

McGowan Method

https://en.wikipedia.org/wiki/Joback_method

NIST Webbook:

<http://link.springer.com/article/10.1007/BF02311772>

Crippen Method:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C111751&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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