

N,N-DIBUTYLETHYLENEDIAMINE

Other names:	2-di-n-Butylaminoethylamine N,N-di-n-Butylethylenediamine 1,2-Ethanediamine, N,N-dibutyl- N,N-Dibutylethylenediamine
Inchi:	InChI=1S/C10H24N2/c1-3-5-8-12(10-7-11)9-6-4-2/h3-11H2,1-2H3
InchiKey:	PWNDYKKNXVKQJO-UHFFFAOYSA-N
Formula:	C10H24N2
SMILES:	CCCCN(CCN)CCCC
Mol. weight [g/mol]:	172.32

Physical Properties

Property code	Value	Unit	Source
af	0.6027		Cheméo Relay (1.0)
gf	210.55	kJ/mol	Joback Method
hf	-183.55	kJ/mol	Cheméo Relay (1.0)
hfus	29.87	kJ/mol	Joback Method
hvap	60.33	kJ/mol	Cheméo Relay (1.0)
ie	8.10	eV	Cheméo Relay (1.0)
log10ws	-1.54		Cheméo Relay (1.0)
logp	1.847		Crippen Method
mcvol	171.720	ml/mol	McGowan Method
pc	2218.71	kPa	Joback Method
tb	488.88	K	Cheméo Relay (1.0)
tc	661.32	K	Cheméo Relay (1.0)
tf	194.63	K	Cheméo Relay (1.0)
vc	0.616	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	417.46	J/mol×K	513.17	Joback Method
cpg	433.48	J/mol×K	541.95	Joback Method
cpg	448.80	J/mol×K	570.73	Joback Method
cpg	463.45	J/mol×K	599.51	Joback Method

cpg	477.44	J/mol×K	628.30	Joback Method
cpg	490.79	J/mol×K	657.08	Joback Method
cpg	503.54	J/mol×K	685.86	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	388.70	K	3.20	NIST Webbook

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C3529097&Units=SI>

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

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

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature

tf: Normal melting (fusion) point
vc: Critical Volume

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