

DIBUTYL-CYANAMIME

Other names:	Di-n-butylcyanamide Dibutylcyanamide N,N-Dibutyl cyanamide
Inchi:	InChI=1S/C9H18N2/c1-3-5-7-11(9-10)8-6-4-2/h3-8H2,1-2H3
InchiKey:	SOGFATPCYLMCMQ-UHFFFAOYSA-N
Formula:	C9H18N2
SMILES:	CCCCN(C#N)CCCC
Mol. weight [g/mol]:	154.26

Physical Properties

Property code	Value	Unit	Source
hf	-19.89	kJ/mol	Cheméo Relay (1.0)
hfus	23.59	kJ/mol	Joback Method
hvap	56.97	kJ/mol	Cheméo Relay (1.0)
ie	8.50	eV	Cheméo Relay (1.0)
log10ws	-2.76		Cheméo Relay (1.0)
logp	2.370		Crippen Method
mcvol	149.030	ml/mol	McGowan Method
pc	2248.26	kPa	Joback Method
tb	516.02	K	Cheméo Relay (1.0)
tc	665.62	K	Cheméo Relay (1.0)
tf	212.35	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	347.90	J/mol×K	519.84	Joback Method
cpg	361.22	J/mol×K	550.04	Joback Method
cpg	373.92	J/mol×K	580.25	Joback Method
cpg	386.03	J/mol×K	610.45	Joback Method
cpg	397.56	J/mol×K	640.65	Joback Method
cpg	408.54	J/mol×K	670.85	Joback Method
cpg	418.99	J/mol×K	701.06	Joback Method

Sources

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=C2050546&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

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