

1-Butanamine, N,N-dipropyl-

Other names:	Butyl di-n-propylamine Butyl dipropyl amine
Inchi:	InChI=1S/C10H23N/c1-4-7-10-11(8-5-2)9-6-3/h4-10H2,1-3H3
InchiKey:	VJIRBKSBKOOVLV-UHFFFAOYSA-N
Formula:	C10H23N
SMILES:	CCCCN(CCC)CCC
Mol. weight [g/mol]:	157.30
CAS:	4444-71-7

Physical Properties

Property code	Value	Unit	Source
gf	144.10	kJ/mol	Joback Method
hf	-182.20	kJ/mol	Joback Method
hfus	24.68	kJ/mol	Joback Method
hvap	39.90	kJ/mol	Joback Method
log10ws	-2.58		Crippen Method
logp	2.909		Crippen Method
mcvol	161.740	ml/mol	McGowan Method
pc	2104.20	kPa	Joback Method
rinpol	1004.00		NIST Webbook
rinpol	1001.00		NIST Webbook
rinpol	1001.00		NIST Webbook
rinpol	1000.30		NIST Webbook
tb	440.64	K	Joback Method
tc	601.86	K	Joback Method
tf	234.93	K	Joback Method
vc	0.614	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	347.57	J/molxK	440.64	Joback Method
cpg	363.50	J/molxK	467.51	Joback Method
cpg	378.81	J/molxK	494.38	Joback Method

cpg	393.52	J/mol×K	521.25	Joback Method
cpg	407.65	J/mol×K	548.12	Joback Method
cpg	421.20	J/mol×K	574.99	Joback Method
cpg	434.20	J/mol×K	601.86	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4444717&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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