

N-Methyl-N-propyl-propylamine

Other names:	1-Propanamine, N-methyl-N-propyl- Methyl di-n-propyl amine Methyl dipropyl amine
Inchi:	InChI=1S/C7H17N/c1-4-6-8(3)7-5-2/h4-7H2,1-3H3
InchiKey:	UVBMZKBIZUWTLV-UHFFFAOYSA-N
Formula:	C7H17N
SMILES:	CCCN(C)CCC
Mol. weight [g/mol]:	115.22
CAS:	3405-42-3

Physical Properties

Property code	Value	Unit	Source
gf	118.84	kJ/mol	Joback Method
hf	-120.28	kJ/mol	Joback Method
hfus	16.91	kJ/mol	Joback Method
hvap	33.22	kJ/mol	Joback Method
log10ws	-1.32		Crippen Method
logp	1.738		Crippen Method
mcvol	119.470	ml/mol	McGowan Method
pc	2793.56	kPa	Joback Method
rinpola	753.00		NIST Webbook
rinpola	757.00		NIST Webbook
rinpola	757.00		NIST Webbook
rinpola	765.00		NIST Webbook
tb	390.15 ± 3.00	K	NIST Webbook
tb	386.65 ± 3.00	K	NIST Webbook
tc	534.55	K	Joback Method
tf	201.12	K	Joback Method
vc	0.446	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	221.39	J/mol×K	372.00	Joback Method

cpg	234.38	J/mol×K	399.09	Joback Method
cpg	246.88	J/mol×K	426.18	Joback Method
cpg	258.89	J/mol×K	453.28	Joback Method
cpg	270.43	J/mol×K	480.37	Joback Method
cpg	281.51	J/mol×K	507.46	Joback Method
cpg	292.14	J/mol×K	534.55	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
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=C3405423&Units=SI

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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