1-Propanamine, N,N,2-trimethyl

Other names:	N,N-Dimethyl isobutylamine
	Isobutylamine, N,N-dimethyl
Inchi:	InChI=1S/C6H15N/c1-6(2)5-7(3)4/h6H,5H2,1-4H3
InchiKey:	GDHRQDYGUDOEIZ-UHFFFAOYSA-N
Formula:	C6H15N
SMILES:	CC(C)CN(C)C
Mol. weight [g/mol]:	101.19
CAS:	7239-24-9

Physical Properties

Property code	Value	Unit	Source
affp	968.70	kJ/mol	NIST Webbook
basg	937.80	kJ/mol	NIST Webbook
gf	107.98	kJ/mol	Joback Method
hf	-104.92	kJ/mol	Joback Method
hfus	10.79	kJ/mol	Joback Method
hvap	30.61	kJ/mol	Joback Method
ie	8.31	eV	NIST Webbook
log10ws	-0.66		Crippen Method
logp	1.204		Crippen Method
mcvol	105.380	ml/mol	McGowan Method
pc	3127.99	kPa	Joback Method
tb	353.15 ± 2.00	K	NIST Webbook
tc	515.03	K	Joback Method
tf	174.85	K	Joback Method
vc	0.384	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	183.67	J/mol×K	348.68	Joback Method
cpg	195.83	J/mol×K	376.41	Joback Method
cpg	207.51	J/mol×K	404.13	Joback Method
cpg	218.74	J/mol×K	431.86	Joback Method

cpg	229.51	J/mol×K	459.58	Joback Method
cpg	239.85	J/mol×K	487.31	Joback Method
cpg	249.76	J/mol×K	515.03	Joback Method

Sources

Crippen Method:	https://www.chemeo.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=C7239249&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

affp:	Proton affinity
basg:	Gas basicity
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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