

N,N-Dimethylvaleramide

Other names:	Pentanamide, N,N-dimethyl- Valeramide, N,N-dimethyl- N,N-Dimethylpentanamide Pentanoic acid, dimethylamide
Inchi:	InChI=1S/C7H15NO/c1-4-5-6-7(9)8(2)3/h4-6H2,1-3H3
InchiKey:	BNODIVYXTGTUPS-UHFFFAOYSA-N
Formula:	C7H15NO
SMILES:	CCCCC(=O)N(C)C
Mol. weight [g/mol]:	129.20
CAS:	6225-06-5

Physical Properties

Property code	Value	Unit	Source
gf	-10.08	kJ/mol	Joback Method
hf	-232.86	kJ/mol	Joback Method
hfus	18.51	kJ/mol	Joback Method
hvap	39.97	kJ/mol	Joback Method
log10ws	-1.10		Crippen Method
logp	1.265		Crippen Method
mcvol	121.040	ml/mol	McGowan Method
pc	2989.32	kPa	Joback Method
tb	425.87	K	Joback Method
tc	600.81	K	Joback Method
tf	251.05	K	Joback Method
vc	0.452	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	244.86	J/molxK	425.87	Joback Method
cpg	257.29	J/molxK	455.03	Joback Method
cpg	269.17	J/molxK	484.18	Joback Method
cpg	280.54	J/molxK	513.34	Joback Method
cpg	291.41	J/molxK	542.50	Joback Method

cpg	301.79	J/mol×K	571.65	Joback Method
cpg	311.69	J/mol×K	600.81	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	378.50 ± 0.50	K	3.30	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6225065&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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
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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