N,N'-Dimethyl valeramide

Other names: N,N-Dimethylpentanamide
Pentanamide, N,N-dimethyl-
Pentanoic acid, dimethylamide
Valeramide, N,N-dimethyl-
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

Physical Properties

Property code	Value	Unit	Source
af	0.4688		Cheméo Relay (1.0)
gf	-10.08	kJ/mol	Joback Method
hf	-292.08	kJ/mol	Cheméo Relay (1.0)
hfus	18.51	kJ/mol	Joback Method
hvap	54.83	kJ/mol	Cheméo Relay (1.0)
ie	8.81	eV	Cheméo Relay (1.0)
log10ws	0.11		Cheméo Relay (1.0)
logp	1.265		Crippen Method
mcvol	121.040	ml/mol	McGowan Method
pc	2989.32	kPa	Joback Method
tb	459.81	K	Cheméo Relay (1.0)
tc	627.85	K	Cheméo Relay (1.0)
tf	237.85	K	Cheméo Relay (1.0)
vc	0.467	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

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

cpg	291.41	J/mol×K	542.50	Joback Method
cpg	301.79	J/mol×K	571.65	Joback Method
cpg	311.69	J/mol×K	600.81	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6225065&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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):

Legend

af: Acentric Factor
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