

Pentanamide, 4-methyl-

Other names:	Valeramide, 4-methyl- «gamma»-Methylvaleramide 4-Methylvaleramide 4-Methyl-N-valeramide
Inchi:	InChI=1S/C6H13NO/c1-5(2)3-4-6(7)8/h5H,3-4H2,1-2H3,(H2,7,8)
InchiKey:	ACMPWZQOUILVFB-UHFFFAOYSA-N
Formula:	C6H13NO
SMILES:	CC(C)CCC(N)=O
Mol. weight [g/mol]:	115.17
CAS:	1119-29-5

Physical Properties

Property code	Value	Unit	Source
gf	-65.27	kJ/mol	Joback Method
hf	-251.24	kJ/mol	Joback Method
hfus	14.57	kJ/mol	Joback Method
hvap	45.95	kJ/mol	Joback Method
log10ws	-1.30		Crippen Method
logp	0.908		Crippen Method
mcvol	106.950	ml/mol	McGowan Method
pc	3602.88	kPa	Joback Method
tb	462.64	K	Joback Method
tc	658.38	K	Joback Method
tf	275.57	K	Joback Method
vc	0.401	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	228.86	J/mol×K	462.64	Joback Method
cpg	239.94	J/mol×K	495.26	Joback Method
cpg	250.51	J/mol×K	527.89	Joback Method
cpg	260.58	J/mol×K	560.51	Joback Method
cpg	270.17	J/mol×K	593.13	Joback Method

cpg	279.28	J/mol×K	625.75	Joback Method
cpg	287.95	J/mol×K	658.38	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1119295&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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