

Gamma,gamma-dimethyl valeramide

Inchi:	InChI=1S/C7H15NO/c1-7(2,3)5-4-6(8)9/h4-5H2,1-3H3,(H2,8,9)
InchiKey:	GNIXIZIBODKFLK-UHFFFAOYSA-N
Formula:	C7H15NO
SMILES:	CC(C)(C)CCC(N)=O
Mol. weight [g/mol]:	129.20
CAS:	15672-96-5

Physical Properties

Property code	Value	Unit	Source
gf	-51.57	kJ/mol	Joback Method
hf	-275.35	kJ/mol	Joback Method
hfus	13.27	kJ/mol	Joback Method
hvap	47.27	kJ/mol	Joback Method
log10ws	-1.72		Crippen Method
logp	1.298		Crippen Method
mcvol	121.040	ml/mol	McGowan Method
pc	3261.58	kPa	Joback Method
tb	482.73	K	Joback Method
tc	684.09	K	Joback Method
tf	304.26	K	Joback Method
vc	0.452	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	273.31	J/molxK	482.73	Joback Method
cpg	286.23	J/molxK	516.29	Joback Method
cpg	298.41	J/molxK	549.85	Joback Method
cpg	309.88	J/molxK	583.41	Joback Method
cpg	320.69	J/molxK	616.97	Joback Method
cpg	330.85	J/molxK	650.53	Joback Method
cpg	340.41	J/molxK	684.09	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C15672965&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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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