

Propanamide, N,2-dimethyl-

Other names:	Propionamide, N,2-dimethyl- N-Methyl-2-methylpropanamide N-Methylisobutyramide
Inchi:	InChI=1S/C5H11NO/c1-4(2)5(7)6-3/h4H,1-3H3,(H,6,7)
InchiKey:	IXHFNEAFAWRVCF-UHFFFAOYSA-N
Formula:	C5H11NO
SMILES:	CNC(=O)C(C)C
Mol. weight [g/mol]:	101.15
CAS:	2675-88-9

Physical Properties

Property code	Value	Unit	Source
basg	873.00 ± 5.00	kJ/mol	NIST Webbook
gf	-50.75	kJ/mol	Joback Method
hf	-210.92	kJ/mol	Joback Method
hfus	11.88	kJ/mol	Joback Method
hvap	67.10 ± 0.20	kJ/mol	NIST Webbook
log10ws	-0.64		Crippen Method
logp	0.388		Crippen Method
mcvol	92.860	ml/mol	McGowan Method
pc	3838.78	kPa	Joback Method
rinpol	940.00		NIST Webbook
rinpol	940.00		NIST Webbook
tb	417.40	K	Joback Method
tc	605.05	K	Joback Method
tf	233.70	K	Joback Method
vc	0.350	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	179.84	J/mol×K	417.40	Joback Method
cpg	189.76	J/mol×K	448.68	Joback Method
cpg	199.25	J/mol×K	479.95	Joback Method

cpg	208.34	J/mol×K	511.23	Joback Method
cpg	217.02	J/mol×K	542.50	Joback Method
cpg	225.31	J/mol×K	573.78	Joback Method
cpg	233.21	J/mol×K	605.05	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2675889&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

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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