

N-(n-Propyl)acetamide

Other names:	Acetamide, N-propyl- N-Propylacetamide Acetamide, N-n-propyl-, N-(n-Propyl)ethanamide
Inchi:	InChI=1S/C5H11NO/c1-3-4-6-5(2)7/h3-4H2,1-2H3,(H,6,7)
InchiKey:	IHPHPGLJYCDONF-UHFFFAOYSA-N
Formula:	C5H11NO
SMILES:	CCCNC(C)=O
Mol. weight [g/mol]:	101.15
CAS:	5331-48-6

Physical Properties

Property code	Value	Unit	Source
gf	-48.31	kJ/mol	Joback Method
hf	-205.64	kJ/mol	Joback Method
hfus	15.40	kJ/mol	Joback Method
hvap	69.80 ± 0.20	kJ/mol	NIST Webbook
log10ws	-0.88		Crippen Method
logp	0.532		Crippen Method
mcvol	92.860	ml/mol	McGowan Method
pc	3801.00	kPa	Joback Method
rinpol	974.00		NIST Webbook
rinpol	974.00		NIST Webbook
rinpol	975.00		NIST Webbook
rinpol	974.00		NIST Webbook
ripol	1802.00		NIST Webbook
ripol	1802.00		NIST Webbook
tb	417.84	K	Joback Method
tc	601.20	K	Joback Method
tf	248.70	K	Joback Method
vc	0.356	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	179.79	J/mol×K	417.84	Joback Method
cpg	189.39	J/mol×K	448.40	Joback Method
cpg	198.59	J/mol×K	478.96	Joback Method
cpg	207.41	J/mol×K	509.52	Joback Method
cpg	215.86	J/mol×K	540.08	Joback Method
cpg	223.93	J/mol×K	570.64	Joback Method
cpg	231.65	J/mol×K	601.20	Joback Method
cpl	207.94	J/mol×K	298.15	NIST Webbook
cpl	207.00	J/mol×K	298.15	NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5331486&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
cpl:	Liquid phase 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
rinpolar:	Non-polar retention indices
ripolar:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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