Acetamide, N-propyl-

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

Physical Properties

Property code	Value	Unit	Source
hf	-306.13	kJ/mol	Cheméo Relay (1.0)
hfus	15.40	kJ/mol	Joback Method
hvap	69.80 ± 0.20	kJ/mol	NIST Webbook
ie	9.29	eV	Cheméo Relay (1.0)
logp	0.532		Crippen Method
mcvol	92.860	ml/mol	McGowan Method
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	449.72	K	Cheméo Relay (1.0)
tf	248.49	K	Cheméo Relay (1.0)

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: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5331486&Units=SI

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

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

Legend

cpg: Ideal gas heat capacity
cpl: Liquid phase heat capacity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tf: Normal melting (fusion) point