

Propanamide, N-propyl-

Inchi:	InChI=1S/C6H13NO/c1-3-5-7-6(8)4-2/h3-5H2,1-2H3,(H,7,8)
InchiKey:	YUMCRXLLWKQDJY-UHFFFAOYSA-N
Formula:	C6H13NO
SMILES:	CCCN=C(O)CC
Mol. weight [g/mol]:	115.17
CAS:	3217-86-5

Physical Properties

Property code	Value	Unit	Source
hf	-246.97	kJ/mol	Joback Method
hvap	49.02	kJ/mol	Joback Method
log10ws	-1.32		Crippen Method
logp	1.763		Crippen Method
mcpol	106.950	ml/mol	McGowan Method
pc	3079.57	kPa	Joback Method
rinpol	1040.00		NIST Webbook
rinpol	1040.00		NIST Webbook
tb	505.42	K	Joback Method
tc	687.80	K	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3217865&Units=SI

Legend

hf: Enthalpy of formation at standard conditions

h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀w_s:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
p_c:	Critical Pressure
r_{inpol}:	Non-polar retention indices
t_b:	Normal Boiling Point Temperature
t_c:	Critical Temperature

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