Propanamide, 2,2-dimethyl-N-ethyl

Other names: Propanamide, N-ethyl-2,2-dimethyl
Inchi: InChI=1S/C7H15NO/c1-5-8-6(9)7(2,3)4/h5H2,1-4H3,(H,8,9)
InchiKey: ICMYVGUJSCZEMG-UHFFFAOYSA-N
Formula: C7H15NO
SMILES: CCNC(=O)C(C)(C)C
Mol. weight [g/mol]: 129.20

Physical Properties

Property code	Value	Unit	Source
gf	-28.63	kJ/mol	Joback Method
hf	-255.67	kJ/mol	Joback Method
hfus	13.17	kJ/mol	Joback Method
hvap	43.06	kJ/mol	Joback Method
log10ws	-1.48		Crippen Method
logp	1.169		Crippen Method
mcvol	121.040	ml/mol	McGowan Method
pc	3103.64	kPa	Joback Method
rinpol	1077.00		NIST Webbook
rinpol	1000.00		NIST Webbook
tb	460.37	K	Joback Method
tc	652.16	K	Joback Method
tf	273.66	K	Joback Method
vc	0.458	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	262.02	J/mol×K	460.37	Joback Method
cpg	275.11	J/mol×K	492.33	Joback Method
cpg	287.51	J/mol×K	524.30	Joback Method
cpg	299.22	J/mol×K	556.26	Joback Method
cpg	310.30	J/mol×K	588.23	Joback Method
cpg	320.75	J/mol×K	620.19	Joback Method
cpg	330.62	J/mol×K	652.16	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R50832&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume