Propanamide, N,N,2-trimethyl

Other names: i-C3H7CON(CH3)2
Inchi: InChI=1S/C6H13NO/c1-5(2)6(8)7(3)4/h5H,1-4H3
InchiKey: GXMIHVHJTLPVKL-UHFFFAOYSA-N
Formula: C6H13NO
SMILES: CC(C)C(=O)N(C)C
Mol. weight [g/mol]: 115.17
CAS: 21678-37-5

Physical Properties

Property code	Value	Unit	Source
affp	923.70	kJ/mol	NIST Webbook
basg	891.80	kJ/mol	NIST Webbook
gf	-20.94	kJ/mol	Joback Method
hf	-217.50	kJ/mol	Joback Method
hfus	12.39	kJ/mol	Joback Method
hvap	37.35	kJ/mol	Joback Method
log10ws	-0.44		Crippen Method
logp	0.731		Crippen Method
mcvol	106.950	ml/mol	McGowan Method
pc	3360.64	kPa	Joback Method
rinpol	959.00		NIST Webbook
rinpol	959.00		NIST Webbook
tb	402.55	K	Joback Method
tc	582.63	K	Joback Method
tf	224.78	K	Joback Method
vc	0.390	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	205.39	J/mol×K	402.55	Joback Method
cpg	217.03	J/mol×K	432.56	Joback Method
cpg	228.16	J/mol×K	462.58	Joback Method
cpg	238.79	J/mol×K	492.59	Joback Method

cpg	248.94	J/mol×K	522.60	Joback Method
cpg	258.61	J/mol×K	552.61	Joback Method
cpg	267.83	J/mol×K	582.63	Joback Method

Sources

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=C21678375&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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