Propanamide, 2-methyl-N-ethyl-N-propyl-

Inchi: InChI=1S/C9H19NO/c1-5-7-10(6-2)9(11)8(3)4/h8H,5-7H2,1-4H3
InchiKey: DGDKJMQJQYPWSY-UHFFFAOYSA-N
Formula: C9H19NO
SMILES: CCCN(CC)C(=O)C(C)C
Mol. weight [g/mol]: 157.25

Physical Properties

Property code	Value	Unit	Source
gf	4.32	kJ/mol	Joback Method
hf	-279.42	kJ/mol	Joback Method
hfus	20.16	kJ/mol	Joback Method
hvap	44.03	kJ/mol	Joback Method
log10ws	-1.69		Crippen Method
logp	1.901		Crippen Method
mcvol	149.220	ml/mol	McGowan Method
pc	2467.81	kPa	Joback Method
rinpol	1272.00		NIST Webbook
rinpol	1272.00		NIST Webbook
tb	471.19	K	Joback Method
tc	647.29	K	Joback Method
tf	258.59	K	Joback Method
vc	0.557	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	330.33	J/mol×K	471.19	Joback Method
cpg	345.04	J/mol×K	500.54	Joback Method
cpg	359.11	J/mol×K	529.89	Joback Method
cpg	372.54	J/mol×K	559.24	Joback Method
cpg	385.37	J/mol×K	588.59	Joback Method
cpg	397.59	J/mol×K	617.94	Joback Method
cpg	409.25	J/mol×K	647.29	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415339&Units=SI

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