Propanamide, N-isopropyl-2-methyl

Inchi: InChI=1S/C7H15NO/c1-5(2)7(9)8-6(3)4/h5-6H,1-4H3,(H,8,9)
InchiKey: IGZDXYHMGWRJAZ-UHFFFAOYSA-N
Formula: C7H15NO
SMILES: CC(C)NC(=O)C(C)C
Mol. weight [g/mol]: 129.20

Physical Properties

Property code	Value	Unit	Source
gf	-36.35	kJ/mol	Joback Method
hf	-257.48	kJ/mol	Joback Method
hfus	13.54	kJ/mol	Joback Method
hvap	43.58	kJ/mol	Joback Method
log10ws	-1.59		Crippen Method
logp	1.167		Crippen Method
mcvol	121.040	ml/mol	McGowan Method
pc	3093.29	kPa	Joback Method
rinpol	987.00		NIST Webbook
tb	462.72	K	Joback Method
tc	651.11	K	Joback Method
tf	241.24	K	Joback Method
vc	0.457	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	259.56	J/mol×K	462.72	Joback Method
cpg	272.19	J/mol×K	494.12	Joback Method
cpg	284.26	J/mol×K	525.52	Joback Method
cpg	295.78	J/mol×K	556.92	Joback Method
cpg	306.77	J/mol×K	588.31	Joback Method
cpg	317.23	J/mol×K	619.71	Joback Method
cpg	327.18	J/mol×K	651.11	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R50971&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

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