Propanamide, N-isobutyl-2,2-dimethyl

Inchi: InChI=1S/C9H19NO/c1-7(2)6-10-8(11)9(3,4)5/h7H,6H2,1-5H3,(H,10,11)
InchiKey: RNMWYCQHYZNXRL-UHFFFAOYSA-N
Formula: C9H19NO
SMILES: CC(C)CNC(=O)C(C)(C)C
Mol. weight [g/mol]: 157.25

Physical Properties

Property code	Value	Unit	Source
gf	-14.23	kJ/mol	Joback Method
hf	-302.23	kJ/mol	Joback Method
hfus	14.83	kJ/mol	Joback Method
hvap	47.13	kJ/mol	Joback Method
log10ws	-2.07		Crippen Method
logp	1.805		Crippen Method
mcvol	149.220	ml/mol	McGowan Method
pc	2553.34	kPa	Joback Method
rinpol	1136.00		NIST Webbook
tb	505.69	K	Joback Method
tc	697.21	K	Joback Method
tf	281.20	K	Joback Method
vc	0.564	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	350.32	J/mol×K	505.69	Joback Method
cpg	365.54	J/mol×K	537.61	Joback Method
cpg	379.95	J/mol×K	569.53	Joback Method
cpg	393.58	J/mol×K	601.45	Joback Method
cpg	406.47	J/mol×K	633.37	Joback Method
cpg	418.64	J/mol×K	665.29	Joback Method
cpg	430.13	J/mol×K	697.21	Joback Method

Sources

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=R50935&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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