Propanamide, 2-methyl-N-ethyl-N-isobutyl-

Inchi: InChI=1S/C10H21NO/c1-6-11(7-8(2)3)10(12)9(4)5/h8-9H,6-7H2,1-5H3
InchiKey: DMNITQKNRDZCRM-UHFFFAOYSA-N
Formula: C10H21NO
SMILES: CCN(CC(C)C)C(=O)C(C)C
Mol. weight [g/mol]: 171.28

Physical Properties

Property code	Value	Unit	Source
gf	10.30	kJ/mol	Joback Method
hf	-305.34	kJ/mol	Joback Method
hfus	19.23	kJ/mol	Joback Method
hvap	45.87	kJ/mol	Joback Method
log10ws	-1.87		Crippen Method
logp	2.147		Crippen Method
mcvol	163.310	ml/mol	McGowan Method
pc	2265.42	kPa	Joback Method
rinpol	1333.00		NIST Webbook
tb	493.63	K	Joback Method
tc	671.86	K	Joback Method
tf	254.86	K	Joback Method
vc	0.608	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	376.20	J/mol×K	493.63	Joback Method
cpg	392.10	J/mol×K	523.33	Joback Method
cpg	407.29	J/mol×K	553.04	Joback Method
cpg	421.77	J/mol×K	582.74	Joback Method
cpg	435.58	J/mol×K	612.45	Joback Method
cpg	448.73	J/mol×K	642.15	Joback Method
cpg	461.25	J/mol×K	671.86	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=U415340&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