Propanamide, N-isobutyl

Inchi: InChI=1S/C7H15NO/c1-4-7(9)8-5-6(2)3/h6H,4-5H2,1-3H3,(H,8,9)
InchiKey: QTVUDNOFBZLOHM-UHFFFAOYSA-N
Formula: C7H15NO
SMILES: CCC(=O)NCC(C)C
Mol. weight [g/mol]: 129.20

Physical Properties

Property code	Value	Unit	Source
gf	-33.91	kJ/mol	Joback Method
hf	-252.20	kJ/mol	Joback Method
hfus	17.06	kJ/mol	Joback Method
hvap	43.97	kJ/mol	Joback Method
log10ws	-1.48		Crippen Method
logp	1.169		Crippen Method
mcvol	121.040	ml/mol	McGowan Method
pc	3065.95	kPa	Joback Method
rinpol	1091.00		NIST Webbook
tb	463.16	K	Joback Method
tc	647.45	K	Joback Method
tf	256.24	K	Joback Method
vc	0.463	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	259.41	J/mol×K	463.16	Joback Method
cpg	271.69	J/mol×K	493.87	Joback Method
cpg	283.44	J/mol×K	524.59	Joback Method
cpg	294.67	J/mol×K	555.30	Joback Method
cpg	305.40	J/mol×K	586.02	Joback Method
cpg	315.63	J/mol×K	616.73	Joback Method
cpg	325.37	J/mol×K	647.45	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=R50921&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