

N-Isopentylformamide

Inchi:	InChI=1S/C6H13NO/c1-6(2)3-4-7-5-8/h5-6H,3-4H2,1-2H3,(H,7,8)
InchiKey:	WRWGCPXFAJKWDW-UHFFFAOYSA-N
Formula:	C6H13NO
SMILES:	CC(C)CCNC=O
Mol. weight [g/mol]:	115.17

Physical Properties

Property code	Value	Unit	Source
gf	-12.93	kJ/mol	Joback Method
hf	-204.56	kJ/mol	Joback Method
hfus	15.16	kJ/mol	Joback Method
hvap	41.72	kJ/mol	Joback Method
log10ws	-1.06		Crippen Method
logp	0.778		Crippen Method
mcvol	106.950	ml/mol	McGowan Method
pc	3464.28	kPa	Joback Method
rinpol	1112.00		NIST Webbook
rinpol	1112.00		NIST Webbook
tb	435.07	K	Joback Method
tc	616.14	K	Joback Method
tf	237.04	K	Joback Method
vc	0.417	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	220.08	J/mol×K	435.07	Joback Method
cpg	230.91	J/mol×K	465.25	Joback Method
cpg	241.29	J/mol×K	495.43	Joback Method
cpg	251.22	J/mol×K	525.61	Joback Method
cpg	260.71	J/mol×K	555.79	Joback Method
cpg	269.78	J/mol×K	585.97	Joback Method
cpg	278.43	J/mol×K	616.14	Joback Method

Sources

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=R508931&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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