N-(3-Methylbutyl)acetamide

Other names:	Acetamide, N-(3-methylbutyl)-
	N-Isopentylacetamide
	Isoamyl acetamide
	N-Isoamylacetamide
	Acetamide, N-isopentyl
Inchi:	InChI=1S/C7H15NO/c1-6(2)4-5-8-7(3)9/h6H,4-5H2,1-3H3,(H,8,9)
InchiKey:	XWDCLPNMPBQWCW-UHFFFAOYSA-N
Formula:	C7H15NO
SMILES:	CC(=O)NCCC(C)C
Mol. weight [g/mol]:	129.20
CAS:	13434-12-3

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	1150.00		NIST Webbook
rinpol	1114.00		NIST Webbook
rinpol	1150.00		NIST Webbook
rinpol	1114.00		NIST Webbook
ripol	1890.00		NIST Webbook
ripol	1816.00		NIST Webbook
ripol	1895.80		NIST Webbook
ripol	1895.80		NIST Webbook
ripol	1890.00		NIST Webbook
ripol	1866.00		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

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=C13434123&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume