Butanamide, N-methyl-

Inchi: InChI=1S/C5H11NO/c1-3-4-5(7)6-2/h3-4H2,1-2H3,(H,6,7)
InchiKey: OLLZXQIFCRIRMH-UHFFFAOYSA-N
Formula: C5H11NO
SMILES: CCCC(O)=NC
Mol. weight [g/mol]: 101.15
CAS: 17794-44-4

Physical Properties

Property code	Value	Unit	Source
hf	-226.33	kJ/mol	Joback Method
hvap	46.80	kJ/mol	Joback Method
ie	9.68 ± 0.05	eV	NIST Webbook
log10ws	-0.90		Crippen Method
logp	1.373		Crippen Method
mcvol	92.860	ml/mol	McGowan Method
pc	3435.91	kPa	Joback Method
rinpol	1005.00		NIST Webbook
rinpol	1005.00		NIST Webbook
tb	482.54	K	Joback Method
tc	666.81	K	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpl	207.00	J/mol×K	298.15	NIST Webbook

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=C17794444&Units=SI

Legend

cpl:	Liquid phase heat capacity
hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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