N-Methylvaleramide

Other names: N-Methylpentanamide
Inchi: InChI=1S/C6H13NO/c1-3-4-5-6(8)7-2/h3-5H2,1-2H3,(H,7,8)
InchiKey: XKEKKGKDCHCOSA-UHFFFAOYSA-N
Formula: C6H13NO
SMILES: CCCCC(O)=NC
Mol. weight [g/mol]: 115.17
CAS: 6225-10-1

Physical Properties

Property code	Value	Unit	Source
hf	-246.97	kJ/mol	Joback Method
hvap	49.02	kJ/mol	Joback Method
log10ws	-1.32		Crippen Method
logp	1.763		Crippen Method
mcvol	106.950	ml/mol	McGowan Method
pc	3079.57	kPa	Joback Method
rinpol	1105.00		NIST Webbook
rinpol	1105.00		NIST Webbook
tb	505.42	K	Joback Method
tc	687.80	K	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpl	238.40	J/mol×K	298.15	NIST Webbook
cpl	229.00	J/mol×K	298.15	NIST Webbook

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=C6225101&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpl:	Liquid phase heat capacity
hf:	Enthalpy of formation 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

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