N,N-Dimethylhexanamide

Other names: Hexanamide, N,N-dimethyl-
N,N-Dimethylcaproamide
Inchi: InChI=1S/C8H17NO/c1-4-5-6-7-8(10)9(2)3/h4-7H2,1-3H3
InchiKey: OAERLTPBKQBWHJ-UHFFFAOYSA-N
Formula: C8H17NO
SMILES: CCCCCC(=O)N(C)C
Mol. weight [g/mol]: 143.23
CAS: 5830-30-8

Physical Properties

Property code	Value	Unit	Source
basg	898.00 ± 5.00	kJ/mol	NIST Webbook
gf	-1.66	kJ/mol	Joback Method
hf	-253.50	kJ/mol	Joback Method
hfus	21.10	kJ/mol	Joback Method
hvap	42.19	kJ/mol	Joback Method
log10ws	-1.52		Crippen Method
logp	1.655		Crippen Method
mcvol	135.130	ml/mol	McGowan Method
pc	2698.60	kPa	Joback Method
tb	448.75	K	Joback Method
tc	622.49	K	Joback Method
tf	262.32	K	Joback Method
vc	0.507	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	286.50	J/mol×K	448.75	Joback Method
cpg	299.93	J/mol×K	477.71	Joback Method
cpg	312.79	J/mol×K	506.66	Joback Method
cpg	325.09	J/mol×K	535.62	Joback Method
cpg	336.84	J/mol×K	564.58	Joback Method
cpg	348.07	J/mol×K	593.54	Joback Method

cpg	358.78	J/mol×K	622.49	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	408.50 ± 0.50	K	0.33	NIST Webbook

Sources

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=C5830308&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

basg: Gas basicity
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
tb: Normal Boiling Point Temperature
tbrp: Boiling point at reduced pressure
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume