N,N-Dimethylbutyramide

Other names:	Butanamide, N,N-dimethyl-
	Butyramide, N,N-dimethyl-
	N,N-Dimethyl-n-butyramide
	N,N-Dimethylbutanamide
Inchi:	InChI=1S/C6H13NO/c1-4-5-6(8)7(2)3/h4-5H2,1-3H3
InchiKey:	VIJUZNJJLALGNJ-UHFFFAOYSA-N
Formula:	C6H13NO
SMILES:	CCCC(=O)N(C)C
Mol. weight [g/mol]:	115.17
CAS:	760-79-2

Physical Properties

Property code	Value	Unit	Source
affp	921.70	kJ/mol	NIST Webbook
basg	890.80	kJ/mol	NIST Webbook
basg	898.00 ± 8.00	kJ/mol	NIST Webbook
chl	-3893.00 ± 1.30	kJ/mol	NIST Webbook
gf	-18.50	kJ/mol	Joback Method
hf	-270.90	kJ/mol	NIST Webbook
hfus	15.92	kJ/mol	Joback Method
hvap	55.19	kJ/mol	NIST Webbook
log10ws	-0.68		Crippen Method
logp	0.875		Crippen Method
mcvol	106.950	ml/mol	McGowan Method
pc	3329.68	kPa	Joback Method
rinpol	978.00		NIST Webbook
tb	402.99	K	Joback Method
tc	578.97	K	Joback Method
tf	239.78	K	Joback Method
vc	0.396	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	205.41	J/mol×K	402.99	Joback Method
cpg	216.70	J/mol×K	432.32	Joback Method
cpg	227.51	J/mol×K	461.65	Joback Method
cpg	237.84	J/mol×K	490.98	Joback Method
cpg	247.72	J/mol×K	520.31	Joback Method
cpg	257.15	J/mol×K	549.64	Joback Method
cpg	266.15	J/mol×K	578.97	Joback Method
hvapt	50.80	kJ/mol	341.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	354.00 ± 1.00	K	2.00	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C760792&Units=SI
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

Legend

affp: Proton affinity
basg: Gas basicity
chl: Standard liquid enthalpy of combustion
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
hvapt: Enthalpy of vaporization at a given temperature
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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