Butanamide, 3-methyl-

Other names:	Isovaleramide
	«beta»-Methylbutyramide
	Isovaleric amide
	3-Methylbutyramide
	3-Methylbutanamide
	3-Methylbutaneamide
	Isopentanamide
Inchi:	InChI=1S/C5H11NO/c1-4(2)3-5(6)7/h4H,3H2,1-2H3,(H2,6,7)
InchiKey:	SANOUVWGPVYVAV-UHFFFAOYSA-N
Formula:	C5H11NO
SMILES:	CC(C)CC(N)=O
Mol. weight [g/mol]:	101.15
CAS:	541-46-8

Physical Properties

Property code	Value	Unit	Source
chs	-3149.70 ± 1.70	kJ/mol	NIST Webbook
gf	-73.69	kJ/mol	Joback Method
hf	-230.60	kJ/mol	Joback Method
hfs	-390.00 ± 1.70	kJ/mol	NIST Webbook
hfus	11.98	kJ/mol	Joback Method
hvap	43.72	kJ/mol	Joback Method
log10ws	-0.88		Crippen Method
logp	0.518		Crippen Method
mcvol	92.860	ml/mol	McGowan Method
pc	4056.96	kPa	Joback Method
ripol	1903.00		NIST Webbook
ripol	1857.00		NIST Webbook
ripol	1903.00		NIST Webbook
ripol	1857.00		NIST Webbook
tb	439.76	K	Joback Method
tc	637.73	K	Joback Method
tf	264.30	K	Joback Method
vc	0.344	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	189.43	J/mol×K	439.76	Joback Method
cpg	199.25	J/mol×K	472.75	Joback Method
cpg	208.63	J/mol×K	505.75	Joback Method
cpg	217.57	J/mol×K	538.74	Joback Method
cpg	226.08	J/mol×K	571.74	Joback Method
cpg	234.18	J/mol×K	604.73	Joback Method
cpg	241.88	J/mol×K	637.73	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C541468&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

chs: Standard solid enthalpy of combustion
cpg: Ideal gas heat capacity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfs: Solid phase 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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point

vc: Critical Volume

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