1-Butanamine, N-methyl-N-nitro-

Other names: Butylmethylnitramine
N-methyl-N-nitrobutanamine
Inchi: InChI=1S/C5H12N2O2/c1-3-4-5-6(2)7(8)9/h3-5H2,1-2H3
InchiKey: USAARNBTXBIFTC-UHFFFAOYSA-N
Formula: C5H12N2O2
SMILES: CCCCN(C)[N+](=O)[O-]
Mol. weight [g/mol]: 132.16
CAS: 52330-07-1

Physical Properties

Property code	Value	Unit	Source
gf	137.55	kJ/mol	Joback Method
hf	-89.76	kJ/mol	Joback Method
hfus	23.09	kJ/mol	Joback Method
hvap	45.36	kJ/mol	Joback Method
log10ws	-1.56		Crippen Method
logp	0.910		Crippen Method
mcvol	108.710	ml/mol	McGowan Method
pc	3509.58	kPa	Joback Method
tb	478.08	K	Joback Method
tc	679.83	K	Joback Method
tf	322.19	K	Joback Method
vc	0.415	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	291.91	J/mol×K	646.20	Joback Method
cpg	239.95	J/mol×K	478.08	Joback Method
cpg	251.55	J/mol×K	511.70	Joback Method
cpg	262.52	J/mol×K	545.33	Joback Method
cpg	272.89	J/mol×K	578.95	Joback Method
cpg	282.67	J/mol×K	612.58	Joback Method
cpg	300.61	J/mol×K	679.83	Joback Method

hfust	37.56	kJ/mol	331.00	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=C52330071&Units=SI

Legend

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
hfust:	Enthalpy of fusion at a given temperature
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume