Butane, 2,3-dimethyl-2,3-dinitro-

Other names:	2,3-Dimethyl-2,3-dinitro-n-butane
	2,3-Dimethyl-2,3-dinitrobutane
	DMNB
	DMNB (2,3-dimethyl-2,3-dinitrobutane)
	dimethyldinitrobutane
Inchi:	InChI=1S/C6H12N2O4/c1-5(2,7(9)10)6(3,4)8(11)12/h1-4H3
InchiKey:	DWCLXOREGBLXTD-UHFFFAOYSA-N
Formula:	C6H12N2O4
SMILES:	CC(C)([N+](=O)[O-])C(C)(C)[N+](=O)[O-]
Mol. weight [g/mol]:	176.17
CAS:	3964-18-9

Physical Properties

Property code	Value	Unit	Source
chs	-3855.10 ± 6.70	kJ/mol	NIST Webbook
chs	-3765.00 ± 1.00	kJ/mol	NIST Webbook
gf	76.42	kJ/mol	Joback Method
hf	-206.19	kJ/mol	Joback Method
hfs	-311.00 ± 1.00	kJ/mol	NIST Webbook
hfus	19.19	kJ/mol	Joback Method
hsub	79.50 ± 0.80	kJ/mol	NIST Webbook
hvap	59.54	kJ/mol	Joback Method
log10ws	-4.17		Aqueous Solubility Prediction Method
logp	1.097		Crippen Method
mcvol	130.240	ml/mol	McGowan Method
pc	3333.53	kPa	Joback Method
rinpol	1126.00		NIST Webbook
rinpol	1154.00		NIST Webbook
rinpol	1128.00		NIST Webbook
tb	633.90	K	Joback Method
tc	891.58	K	Joback Method
tf	449.44	K	Joback Method
vc	0.513	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	371.49	J/mol×K	719.79	Joback Method
cpg	360.36	J/mol×K	676.85	Joback Method
cpg	406.96	J/mol×K	891.58	Joback Method
cpg	399.22	J/mol×K	848.63	Joback Method
cpg	390.80	J/mol×K	805.69	Joback Method
cpg	381.60	J/mol×K	762.74	Joback Method
cpg	348.09	J/mol×K	633.90	Joback Method
hfust	8.80	kJ/mol	473.00	NIST Webbook
hsubt	85.00 ± 2.00	kJ/mol	316.50	NIST Webbook
psub	1.13e-03	kPa	313.00	Aliphatic nitroalkanes: Evaluation of thermochemical data with complementary experimental and computational methods
psub	2.20e-04	kPa	298.20	Aliphatic nitroalkanes: Evaluation of thermochemical data with complementary experimental and computational methods
psub	2.30e-04	kPa	298.20	Aliphatic nitroalkanes: Evaluation of thermochemical data with complementary experimental and computational methods
psub	3.80e-04	kPa	303.20	Aliphatic nitroalkanes: Evaluation of thermochemical data with complementary experimental and computational methods

psub	4.20e-04	kPa	303.20	Aliphatic nitroalkanes: Evaluation of thermochemical data with complementary experimental and computational methods
psub	6.60e-04	kPa	308.10	Aliphatic nitroalkanes: Evaluation of thermochemical data with complementary experimental and computational methods
psub	7.10e-04	kPa	308.20	Aliphatic nitroalkanes: Evaluation of thermochemical data with complementary experimental and computational methods
psub	1.20e-04	kPa	293.40	Aliphatic nitroalkanes: Evaluation of thermochemical data with complementary experimental and computational methods
psub	1.13e-03	kPa	313.00	Aliphatic nitroalkanes: Evaluation of thermochemical data with complementary experimental and computational methods
psub	1.25e-03	kPa	313.20	Aliphatic nitroalkanes: Evaluation of thermochemical data with complementary experimental and computational methods
psub	1.99e-03	kPa	318.00	Aliphatic nitroalkanes: Evaluation of thermochemical data with complementary experimental and computational methods

psub	2.06e-03	kPa	318.00	Aliphatic nitroalkanes: Evaluation of thermochemical data with complementary experimental and computational methods
psub	1.90e-03	kPa	318.20	Aliphatic nitroalkanes: Evaluation of thermochemical data with complementary experimental and computational methods
psub	2.05e-03	kPa	318.20	Aliphatic nitroalkanes: Evaluation of thermochemical data with complementary experimental and computational methods
psub	1.30e-04	kPa	293.30	Aliphatic nitroalkanes: Evaluation of thermochemical data with complementary experimental and computational methods
psub	1.20e-04	kPa	293.20	Aliphatic nitroalkanes: Evaluation of thermochemical data with complementary experimental and computational methods
psub	6.00e-05	kPa	288.30	Aliphatic nitroalkanes: Evaluation of thermochemical data with complementary experimental and computational methods
psub	7.00e-05	kPa	288.30	Aliphatic nitroalkanes: Evaluation of thermochemical data with complementary experimental and computational methods

psub	3.00e-05	kPa	283.30	Aliphatic nitroalkanes: Evaluation of thermochemical data with complementary experimental and computational methods
psub	4.00e-05	kPa	283.30	Aliphatic nitroalkanes: Evaluation of thermochemical data with complementary experimental and computational methods
psub	3.00e-05	kPa	283.30	Aliphatic nitroalkanes: Evaluation of thermochemical data with complementary experimental and computational methods
psub	4.00e-05	kPa	283.30	Aliphatic nitroalkanes: Evaluation of thermochemical data with complementary experimental and computational methods
psub	2.00e-05	kPa	278.40	Aliphatic nitroalkanes: Evaluation of thermochemical data with complementary experimental and computational methods

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.69113e+01
Coeff. B	-5.42634e+03
Coeff. C	-8.95050e+01
Temperature range (K), min.	415.93

Temperature range (K), max.	557.30

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3964189&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Aliphatic nitroalkanes: Evaluation of thermochemical data with complementary experimental and computational methods:	https://www.doi.org/10.1016/j.tca.2017.07.001
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
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
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation 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
psub:	Sublimation pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume