Butane, 1-nitro-

Other names: 1-Nitrobutane
Nitro-butane
n-C4H9NO2
Inchi: InChI=1S/C4H9NO2/c1-2-3-4-5(6)7/h2-4H2,1H3
InchiKey: NALZTFARIYUCBY-UHFFFAOYSA-N
Formula: C4H9NO2
SMILES: CCCC[N+](=O)[O-]
Mol. weight [g/mol]: 103.12
CAS: 627-05-4

Physical Properties

Property code	Value	Unit	Source
af	0.4520		KDB
chl	-2667.80 ± 1.30	kJ/mol	NIST Webbook
gf	18.35	kJ/mol	Joback Method
hf	-136.65	kJ/mol	Joback Method
hfl	-192.60 ± 1.30	kJ/mol	NIST Webbook
hfus	17.48	kJ/mol	Joback Method
hvap	48.58 ± 0.50	kJ/mol	NIST Webbook
hvap	47.00	kJ/mol	NIST Webbook
ie	10.71 ± 0.01	eV	NIST Webbook
log10ws	-1.58		Crippen Method
logp	1.063		Crippen Method
mcvol	84.640	ml/mol	McGowan Method
pc	3800.00	kPa	KDB
rinpol	808.56		NIST Webbook
rinpol	804.00		NIST Webbook
rinpol	791.00		NIST Webbook
rinpol	805.00		NIST Webbook
rinpol	805.00		NIST Webbook
rinpol	804.00		NIST Webbook
rinpol	842.53		NIST Webbook
rinpol	826.02		NIST Webbook
rinpol	826.02		NIST Webbook
rinpol	810.11		NIST Webbook
rinpol	811.95		NIST Webbook
rinpol	801.32		NIST Webbook

rinpol	802.43		NIST Webbook
rinpol	803.51		NIST Webbook
rinpol	804.40		NIST Webbook
rinpol	805.74		NIST Webbook
rinpol	807.39		NIST Webbook
rinpol	763.80		NIST Webbook
rinpol	853.48		NIST Webbook
rinpol	765.20		NIST Webbook
rinpol	767.00		NIST Webbook
rinpol	824.00		NIST Webbook
rinpol	824.00		NIST Webbook
rinpol	822.00		NIST Webbook
rinpol	754.60		NIST Webbook
rinpol	788.00		NIST Webbook
rinpol	804.00		NIST Webbook
rinpol	791.00		NIST Webbook
rinpol	800.00		NIST Webbook
rinpol	791.00		NIST Webbook
ripol	1337.10		NIST Webbook
ripol	1317.50		NIST Webbook
ripol	1331.20		NIST Webbook
ripol	1326.60		NIST Webbook
ripol	1331.20		NIST Webbook
ripol	1322.00		NIST Webbook
ripol	1333.70		NIST Webbook
ripol	1313.50		NIST Webbook
ripol	1310.20		NIST Webbook
ripol	1317.50		NIST Webbook
tb	426.10	K	KDB
tb	425.92 ± 0.06	K	NIST Webbook
tb	427.05 ± 0.50	K	NIST Webbook
tb	426.10 ± 0.70	K	NIST Webbook
tb	426.20	K	NIST Webbook
tc	624.00	K	KDB
tf	191.82 ± 0.05	K	NIST Webbook
tf	192.00	K	KDB
vc	0.342	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	170.19	J/mol×K	442.76	Joback Method
cpg	179.46	J/mol×K	477.27	Joback Method
cpg	188.26	J/mol×K	511.77	Joback Method
cpg	196.63	J/mol×K	546.28	Joback Method
cpg	204.56	J/mol×K	580.78	Joback Method
cpg	212.08	J/mol×K	615.29	Joback Method
cpg	219.20	J/mol×K	649.80	Joback Method
hvapt	38.91	kJ/mol	426.10	KDB
hvapt	42.70	kJ/mol	391.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.67422e+01
Coeff. B	-5.64585e+03
Coeff. C	3.94820e+01
Temperature range (K), min.	303.64
Temperature range (K), max.	454.44

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.64654e+02
Coeff. B	-1.17644e+04
Coeff. C	-2.23635e+01
Coeff. D	1.65370e-05
Temperature range (K), min.	279.15
Temperature range (K), max.	624.00

Sources

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1434
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
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1434
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C627054&Units=SI

Legend

af:	Acentric Factor
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
hfl:	Liquid phase 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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume