Butane, 2-nitro-

Other names: 2-Nitrobutane
sec-C4H9NO2
Inchi: InChI=1S/C4H9NO2/c1-3-4(2)5(6)7/h4H,3H2,1-2H3
InchiKey: SUGZATOHBPXTDV-UHFFFAOYSA-N
Formula: C4H9NO2
SMILES: CCC(C)[N+](=O)[O-]
Mol. weight [g/mol]: 103.12
CAS: 600-24-8

Physical Properties

Property code	Value	Unit	Source
af	0.3570		KDB
chl	-2652.70 ± 1.50	kJ/mol	NIST Webbook
gf	15.91	kJ/mol	Joback Method
hf	-141.93	kJ/mol	Joback Method
hfl	-207.60 ± 1.50	kJ/mol	NIST Webbook
hfus	13.95	kJ/mol	Joback Method
hvap	43.85 ± 0.42	kJ/mol	NIST Webbook
ie	10.71 ± 0.01	eV	NIST Webbook
log10ws	-1.69		Crippen Method
logp	1.062		Crippen Method
mcvol	84.640	ml/mol	McGowan Method
pc	3600.00	kPa	KDB
rinpol	776.00		NIST Webbook
rinpol	774.00		NIST Webbook
rinpol	776.00		NIST Webbook
rinpol	776.00		NIST Webbook
tb	412.90	K	KDB
tb	412.80 ± 0.70	K	NIST Webbook
tc	615.00	K	KDB
tf	141.00	K	KDB
tf	412.65 ± 0.07	K	NIST Webbook
vc	0.336	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	170.34	J/mol×K	442.32	Joback Method
cpg	179.92	J/mol×K	477.66	Joback Method
cpg	189.01	J/mol×K	513.00	Joback Method
cpg	197.63	J/mol×K	548.34	Joback Method
cpg	205.79	J/mol×K	583.68	Joback Method
cpg	213.51	J/mol×K	619.02	Joback Method
cpg	220.79	J/mol×K	654.36	Joback Method
hvapt	36.82	kJ/mol	412.90	KDB
hvapt	40.30	kJ/mol	379.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.51998e+01
Coeff. B	-4.19718e+03
Coeff. C	-1.61470e+01
Temperature range (K), min.	297.61
Temperature range (K), max.	440.60

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	3.88020e+01
Coeff. B	-5.62246e+03
Coeff. C	-3.49067e+00
Coeff. D	2.13481e-06
Temperature range (K), min.	348.15
Temperature range (K), max.	615.00

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
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1435
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C600248&Units=SI
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=1435

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume