

3-NITRO-2-BUTANOL

Other names:	2-Butanol, 3-nitro- 2-Nitrobutan-3-ol 3-nitrobutan-2-ol
Inchi:	InChI=1S/C4H9NO3/c1-3(4(2)6)5(7)8/h3-4,6H,1-2H3
InchiKey:	OJVOGABFNZDOOZ-UHFFFAOYSA-N
Formula:	C4H9NO3
SMILES:	CC(O)C(C)[N+](=O)[O-]
Mol. weight [g/mol]:	119.12

Physical Properties

Property code	Value	Unit	Source
af	0.5574		Cheméo Relay (1.0)
chl	-2470.10 ± 4.80	kJ/mol	NIST Webbook
hfl	-390.30 ± 4.80	kJ/mol	NIST Webbook
hfus	14.52	kJ/mol	Joback Method
hvap	61.83	kJ/mol	Cheméo Relay (1.0)
ie	10.71	eV	Cheméo Relay (1.0)
log10ws	-0.05		Cheméo Relay (1.0)
logp	0.032		Crippen Method
mcvol	90.510	ml/mol	McGowan Method
pc	4553.06	kPa	Joback Method
tb	467.59	K	Cheméo Relay (1.0)
tc	661.82	K	Cheméo Relay (1.0)
tf	298.95	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	210.96	J/mol×K	534.06	Joback Method
cpg	219.34	J/mol×K	567.89	Joback Method
cpg	227.26	J/mol×K	601.73	Joback Method
cpg	234.75	J/mol×K	635.56	Joback Method
cpg	241.82	J/mol×K	669.40	Joback Method
cpg	248.47	J/mol×K	703.23	Joback Method

cpg

254.74

J/mol×K

737.07

Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	328.20	K	0.07	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6270162&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point

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