1-Butanol, 2-nitro-

Other names: 2-Nitro-1-butanol
2-Nitrobutanol
2-nitrobutan-1-ol
Inchi: InChI=1S/C4H9NO3/c1-2-4(3-6)5(7)8/h4,6H,2-3H2,1H3
InchiKey: MHIHRIPETCJEMQ-UHFFFAOYSA-N
Formula: C4H9NO3
SMILES: CCC(CO)[N+](=O)[O-]
Mol. weight [g/mol]: 119.12
CAS: 609-31-4

Physical Properties

Property code	Value	Unit	Source
gf	-120.91	kJ/mol	Joback Method
hf	-294.16	kJ/mol	Joback Method
hfus	18.04	kJ/mol	Joback Method
hvap	57.38	kJ/mol	Joback Method
log10ws	-0.96		Crippen Method
logp	0.034		Crippen Method
mcvol	90.510	ml/mol	McGowan Method
pc	4504.30	kPa	Joback Method
ripol	2067.00		NIST Webbook
tb	534.50	K	Joback Method
tc	733.24	K	Joback Method
tf	324.27	K	Joback Method
vc	0.354	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	210.58	J/mol×K	534.50	Joback Method
cpg	218.72	J/mol×K	567.62	Joback Method
cpg	226.43	J/mol×K	600.75	Joback Method
cpg	233.73	J/mol×K	633.87	Joback Method
cpg	240.63	J/mol×K	667.00	Joback Method

cpg	247.16	J/mol×K	700.12	Joback Method
cpg	253.31	J/mol×K	733.24	Joback Method

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=C609314&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
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume