1-Propanol, 2-methyl-2-nitro-

Other names:	2-Nitro-2-methylpropanol
	2-Methyl-2-nitro-1-propanol
	2-Nitro-2-methyl-1-propanol
	2-Methyl-2-nitropropanol
	NMP
	2-methyl-2-nitropropan-1-ol
Inchi:	InChI=1S/C4H9NO3/c1-4(2,3-6)5(7)8/h6H,3H2,1-2H3
InchiKey:	MVGJRISPEUZYAQ-UHFFFAOYSA-N
Formula:	C4H9NO3
SMILES:	CC(C)(CO)[N+](=O)[O-]
Mol. weight [g/mol]:	119.12
CAS:	76-39-1

Physical Properties

Property code	Value	Unit	Source
gf	-115.63	kJ/mol	Joback Method
hf	-297.63	kJ/mol	Joback Method
hfus	14.15	kJ/mol	Joback Method
hvap	56.47	kJ/mol	Joback Method
log10ws	-0.96		Crippen Method
logp	0.034		Crippen Method
mcvol	90.510	ml/mol	McGowan Method
pc	4571.55	kPa	Joback Method
ripol	1898.00		NIST Webbook
tb	531.71	K	Joback Method
tc	738.33	K	Joback Method
tf	341.69	K	Joback Method
vc	0.349	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	214.06	J/mol×K	531.71	Joback Method
cpg	222.56	J/mol×K	566.15	Joback Method

cpg	230.49	J/mol×K	600.58	Joback Method
cpg	237.89	J/mol×K	635.02	Joback Method
cpg	244.78	J/mol×K	669.46	Joback Method
cpg	251.21	J/mol×K	703.90	Joback Method
cpg	257.20	J/mol×K	738.33	Joback Method

Sources

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=C76391&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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