

2-Nitro-2-methyl-1,3-propanediol

Other names:	2-Methyl-2-nitro-1,3-propanediol 1,3-Propanediol, 2-methyl-2-nitro- Nitroisobutylglycol NMPD 1,1-Dimethylol-1-nitroethane 2-Methyl-2-nitropropane-1,3-diol 2-Methyl-2-nitropropanediol NSC 5372
Inchi:	InChI=1S/C4H9NO4/c1-4(2-6,3-7)5(8)9/h6-7H,2-3H2,1H3
InchiKey:	LOTYADDQWWVBDJ-UHFFFAOYSA-N
Formula:	C4H9NO4
SMILES:	CC(CO)(CO)[N+](=O)[O-]
Mol. weight [g/mol]:	135.12
CAS:	77-49-6

Physical Properties

Property code	Value	Unit	Source
chs	-2294.20	kJ/mol	NIST Webbook
chs	-2280.30 ± 2.80	kJ/mol	NIST Webbook
chs	-2289.80 ± 2.30	kJ/mol	NIST Webbook
gf	-252.45	kJ/mol	Joback Method
hf	-449.86	kJ/mol	Joback Method
hfs	-570.50 ± 2.30	kJ/mol	NIST Webbook
hfs	-566.10	kJ/mol	NIST Webbook
hfs	-580.10 ± 2.80	kJ/mol	NIST Webbook
hfus	18.24	kJ/mol	Joback Method
hvap	73.15	kJ/mol	Joback Method
log10ws	-0.22		Crippen Method
logp	-0.994		Crippen Method
mcvol	96.380	ml/mol	McGowan Method
pc	5198.13	kPa	Joback Method
tb	623.89	K	Joback Method
tc	817.70	K	Joback Method
tf	424.00 ± 4.00	K	NIST Webbook
vc	0.368	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	252.59	J/mol×K	623.89	Joback Method
cpg	259.45	J/mol×K	656.19	Joback Method
cpg	265.86	J/mol×K	688.49	Joback Method
cpg	271.86	J/mol×K	720.79	Joback Method
cpg	277.47	J/mol×K	753.10	Joback Method
cpg	282.72	J/mol×K	785.40	Joback Method
cpg	287.65	J/mol×K	817.70	Joback Method
hfust	3.84	kJ/mol	424.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C77496&Units=SI
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

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

tf: Normal melting (fusion) point
vc: Critical Volume

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