

Benzenemethanol, 4-nitro-

Other names:	Benzyl alcohol, p-nitro- p-Nitrobenzyl alcohol 4-Nitrobenzyl alcohol p-(Hydroxymethyl)nitrobenzene 4-NO ₂ -C ₆ H ₄ CH ₂ OH
Inchi:	InChI=1S/C7H7NO3/c9-5-6-1-3-7(4-2-6)8(10)11/h1-4,9H,5H2
InchiKey:	JKTYGPATCNUWKN-UHFFFAOYSA-N
Formula:	C ₇ H ₇ NO ₃
SMILES:	O=[N+](O)c1ccc(CO)cc1
Mol. weight [g/mol]:	153.14
CAS:	619-73-8

Physical Properties

Property code	Value	Unit	Source
affp	810.50	kJ/mol	NIST Webbook
basg	778.00	kJ/mol	NIST Webbook
gf	9.57	kJ/mol	Joback Method
hf	-125.74	kJ/mol	Joback Method
hfus	22.99	kJ/mol	Joback Method
hvap	67.38	kJ/mol	Joback Method
log10ws	-2.27		Crippen Method
logp	1.087		Crippen Method
mvol	109.020	ml/mol	McGowan Method
pc	4627.70	kPa	Joback Method
tb	635.24	K	Joback Method
tc	863.19	K	Joback Method
tf	412.02	K	Joback Method
vc	0.420	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	262.07	J/molxK	635.24	Joback Method
cpg	270.91	J/molxK	673.23	Joback Method

cpg	279.10	J/mol×K	711.22	Joback Method
cpg	286.68	J/mol×K	749.21	Joback Method
cpg	293.68	J/mol×K	787.21	Joback Method
cpg	300.14	J/mol×K	825.20	Joback Method
cpg	306.09	J/mol×K	863.19	Joback Method
hfust	20.97	kJ/mol	237.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	458.20	K	1.60	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C619738&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

affp:	Proton affinity
basg:	Gas basicity
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
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

tbrp: Boiling point at reduced pressure
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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