Benzenemethanol, 3-nitro-

Other names:	Benzyl alcohol, m-nitro-
	m-Nitrobenzyl alcohol
	3-Nitrobenzyl alcohol
	(3-Nitrophenyl) methanol
Inchi:	InChI=1S/C7H7NO3/c9-5-6-2-1-3-7(4-6)8(10)11/h1-4,9H,5H2
InchiKey:	CWNPOQFCIIFQDM-UHFFFAOYSA-N
Formula:	C7H7NO3
SMILES:	O=[N+]([O-])c1cccc(CO)c1
Mol. weight [g/mol]:	153.14
CAS:	619-25-0

Physical Properties

Property code	Value	Unit	Source
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
mcvol	109.020	ml/mol	McGowan Method
pc	4627.70	kPa	Joback Method
rinpol	1545.00		NIST Webbook
tb	635.24	K	Joback Method
tc	863.19	K	Joback Method
tf	412.02	K	Joback Method
vc	0.420	m3/kmol	Joback Method

Temperature Dependent Properties

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

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	450.70	K	0.40	NIST Webbook

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=C619250&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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tbrp: Boiling point at reduced pressure
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume