Benzene, (nitromethyl)-

Other names:	Toluene, «alpha»-nitro- «alpha»-Nitrotoluene (Nitromethyl)benzene Nitrophenylmethane Phenylnitromethane
Inchi:	InChI=1S/C7H7NO2/c9-8(10)6-7-4-2-1-3-5-7/h1-5H,6H2
InchiKey:	VLZLOWPYUQHHCG-UHFFFAOYSA-N
Formula:	C7H7NO2
SMILES:	O=[N+]([O-])Cc1ccccc1
Mol. weight [g/mol]:	137.14
CAS:	622-42-4

Physical Properties

Property code	Value	Unit	Source
chl	-3732.10 ± 2.50	kJ/mol	NIST Webbook
ea	0.65 ± 0.01	eV	NIST Webbook
gf	156.02	kJ/mol	Joback Method
hf	30.70 ± 2.80	kJ/mol	NIST Webbook
hfl	-22.80 ± 2.60	kJ/mol	NIST Webbook
hfus	19.29	kJ/mol	Joback Method
hvap	54.00 ± 1.00	kJ/mol	NIST Webbook
log10ws	-2.44		Crippen Method
logp	1.463		Crippen Method
mcvol	103.150	ml/mol	McGowan Method
pc	4178.49	kPa	Joback Method
rinpol	1152.00		NIST Webbook
tb	499.20	K	NIST Webbook
tc	786.81	K	Joback Method
tf	338.68	K	Joback Method
vc	0.402	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	271.25	J/mol×K	745.36	Joback Method
cpg	222.18	J/mol×K	538.08	Joback Method
cpg	233.70	J/mol×K	579.54	Joback Method
cpg	244.31	J/mol×K	620.99	Joback Method
cpg	254.08	J/mol×K	662.45	Joback Method
cpg	263.04	J/mol×K	703.90	Joback Method
cpg	278.75	J/mol×K	786.81	Joback Method
hvapt	53.80	kJ/mol	388.00	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C622424&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

chl: Standard liquid enthalpy of combustion
cpg: Ideal gas heat capacity
ea: Electron affinity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfl: Liquid phase enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
hvapt: Enthalpy of vaporization at a given temperature
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
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume