

Benzene, 1-(bromomethyl)-4-nitro-

Other names:	Toluene, «alpha»-bromo-p-nitro- «alpha»-Bromo-p-nitrotoluene «alpha»-Bromo-4-nitrotoluene p-Nitrobenzyl bromide Toluene, «alpha»-bromo-4-nitro- 4-Nitrobenzyl bromide «alpha»-Bromoparanitrotoluene p-(Bromomethyl)nitrobenzene 4-(Bromomethyl)nitrobenzene NSC 4609
Inchi:	InChI=1S/C7H6BrNO2/c8-5-6-1-3-7(4-2-6)9(10)11/h1-4H,5H2
InchiKey:	VOLRSQPSJGXRNJ-UHFFFAOYSA-N
Formula:	C7H6BrNO2
SMILES:	O=[N+](O-)[c1ccc(CBr)cc1]
Mol. weight [g/mol]:	216.03
CAS:	100-11-8

Physical Properties

Property code	Value	Unit	Source
gf	160.71	kJ/mol	Joback Method
hf	52.82	kJ/mol	Joback Method
hfus	24.18	kJ/mol	Joback Method
hvap	57.14	kJ/mol	Joback Method
log10ws	-3.43		Crippen Method
logp	2.490		Crippen Method
mcvol	120.650	ml/mol	McGowan Method
pc	4486.22	kPa	Joback Method
tb	609.22	K	Joback Method
tc	873.25	K	Joback Method
tf	372.70 ± 2.00	K	NIST Webbook
vc	0.464	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	251.36	J/mol×K	609.22	Joback Method
cpg	261.26	J/mol×K	653.23	Joback Method
cpg	270.29	J/mol×K	697.23	Joback Method
cpg	278.52	J/mol×K	741.24	Joback Method
cpg	286.01	J/mol×K	785.24	Joback Method
cpg	292.84	J/mol×K	829.25	Joback Method
cpg	299.06	J/mol×K	873.25	Joback Method

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=C100118&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
mccvol:	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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