Benzene, 1-(bromomethyl)-3-nitro-

Other names:	m-(Bromomethyl)nitrobenzene
	«alpha»-Bromo-m-nitrotoluene
	m-Nitrobenzyl bromide
	3-Nitrobenzyl bromide
	m-Nitro-«alpha»-bromotoluene
	Toluene, «alpha»-bromo-m-nitro-
	«alpha»-bromo-3-nitrotoluene
Inchi:	InChI=1S/C7H6BrNO2/c8-5-6-2-1-3-7(4-6)9(10)11/h1-4H,5H2
InchiKey:	LNWXALCHPJANMJ-UHFFFAOYSA-N
Formula:	C7H6BrNO2
SMILES:	O=[N+]([O-])c1cccc(CBr)c1
Mol. weight [g/mol]:	216.03
CAS:	3958-57-4

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	411.00	K	Joback Method
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

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	426.70	K	1.00	NIST Webbook

Sources

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=C3958574&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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