2-Nitrobenzyl bromide

Other names:	o-Nitrobenzyl bromide
	Benzene, 1-(bromomethyl)-2-nitro-
	«alpha»-bromo-2-nitrotoluene
Inchi:	InChI=1S/C7H6BrNO2/c8-5-6-3-1-2-4-7(6)9(10)11/h1-4H,5H2
InchiKey:	HXBMIQJOSHZCFX-UHFFFAOYSA-N
Formula:	C7H6BrNO2
SMILES:	O=[N+]([O-])c1ccccc1CBr
Mol. weight [g/mol]:	216.03
CAS:	3958-60-9

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

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3958609&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

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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume