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

Physical Properties

Property code	Value	Unit	Source
hf	55.34	kJ/mol	Cheméo Relay (1.0)
hfus	24.18	kJ/mol	Joback Method
hvap	68.80	kJ/mol	Cheméo Relay (1.0)
ie	9.78	eV	Cheméo Relay (1.0)
log10ws	-3.16		Cheméo Relay (1.0)
logp	2.490		Crippen Method
mcvol	120.650	ml/mol	McGowan Method
tb	557.57	K	Cheméo Relay (1.0)
tf	337.98	K	Cheméo Relay (1.0)

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
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3958609&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point