p-Bromophenylacetonitrile

Other names:	2-(4-Bromophenyl)acetonitrile
	4-Bromobenzeneacetonitrile
	4-Bromobenzylcyanide
	4-Bromophenylacetonitrile
	Acetonitrile, (p-bromophenyl)-
	NSC 84174
	p-Bromobenzyl cyanide
	p-Bromophenylacetonitrile
Inchi:	InChI=1S/C8H6BrN/c9-8-3-1-7(2-4-8)5-6-10/h1-4H,5H2
InchiKey:	MFHFWRBXPQDZSA-UHFFFAOYSA-N
Formula:	C8H6BrN
SMILES:	N#CCc1ccc(Br)cc1
Mol. weight [g/mol]:	196.05

Physical Properties

Property code	Value	Unit	Source
hfus	16.92	kJ/mol	Joback Method
hvap	71.59	kJ/mol	Cheméo Relay (1.0)
ie	9.23	eV	Cheméo Relay (1.0)
log10ws	-3.21		Cheméo Relay (1.0)
logp	2.515		Crippen Method
mcvol	118.700	ml/mol	McGowan Method
tb	544.28	K	Cheméo Relay (1.0)
tf	343.78	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	230.81	J/mol×K	582.34	Joback Method
cpg	239.86	J/mol×K	623.60	Joback Method
cpg	248.22	J/mol×K	664.87	Joback Method
cpg	255.92	J/mol×K	706.13	Joback Method
cpg	263.01	J/mol×K	747.39	Joback Method
cpg	269.55	J/mol×K	788.66	Joback Method

cpg	275.58	J/mol×K	829.92	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16532799&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
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):	

Legend

cpg:	Ideal gas heat capacity
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