Benzeneacetonitrile, 4-bromo-

Other names:	Acetonitrile, (p-bromophenyl)-
	p-Bromophenylacetonitrile
	2-(4-Bromophenyl)acetonitrile
	4-Bromobenzeneacetonitrile
	4-Bromobenzylcyanide
	4-Bromophenylacetonitrile
	p-Bromobenzyl cyanide
	NSC 84174
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]:	196.04
CAS:	16532-79-9

Physical Properties

Property code	Value	Unit	Source
gf	266.76	kJ/mol	Joback Method
hf	207.82	kJ/mol	Joback Method
hfus	16.92	kJ/mol	Joback Method
hvap	53.25	kJ/mol	Joback Method
log10ws	-3.30		Crippen Method
logp	2.515		Crippen Method
mcvol	118.700	ml/mol	McGowan Method
pc	3782.33	kPa	Joback Method
tb	582.34	K	Joback Method
tc	829.92	K	Joback Method
tf	343.65	K	Joback Method
vc	0.464	m3/kmol	Joback Method

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

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=C16532799&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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume