2-BROMOPHENYLACETONITRILE

Other names:	2-Bromobenzyl cyanide Benzeneacetonitrile, 2-bromo- Acetonitrile, (o-bromophenyl)- o-Bromobenzyl cyanide UN 1694
Inchi:	InChI=1S/C8H6BrN/c9-8-4-2-1-3-7(8)5-6-10/h1-4H,5H2
InchiKey:	BVCOJESIQPNOIF-UHFFFAOYSA-N
Formula:	C8H6BrN
SMILES:	N#CCc1ccccc1Br
Mol. weight [g/mol]:	196.05

Physical Properties

Property code	Value	Unit	Source
hfus	16.92	kJ/mol	Joback Method
hvap	70.56	kJ/mol	Cheméo Relay (1.0)
ie	9.34	eV	Cheméo Relay (1.0)
log10ws	-3.02		Cheméo Relay (1.0)
logp	2.515		Crippen Method
mcvol	118.700	ml/mol	McGowan Method
tb	542.51	K	Cheméo Relay (1.0)
tf	325.78	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

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	413.70	K	1.70	NIST Webbook

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C19472743&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

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
tbrp: Boiling point at reduced pressure
tf: Normal melting (fusion) point