4-BROMOPHENYL ISOCYANATE

Other names:	p-Bromophenylisocyanate
	Isocyanic acid p-bromophenyl ester
	Benzene, 1-bromo-4-isocyanato-
	p-Bromocarbanil
	p-Bromophenyl carbonimide
Inchi:	InChI=1S/C7H4BrNO/c8-6-1-3-7(4-2-6)9-5-10/h1-4H
InchiKey:	CZQIJQFTRGDODI-UHFFFAOYSA-N
Formula:	C7H4BrNO
SMILES:	O=C=Nc1ccc(Br)cc1
Mol. weight [g/mol]:	198.02

Physical Properties

Property code	Value	Unit	Source
hf	31.00	kJ/mol	Cheméo Relay (1.0)
hvap	54.41	kJ/mol	Cheméo Relay (1.0)
ie	8.65	eV	Cheméo Relay (1.0)
log10ws	-3.23		Cheméo Relay (1.0)
logp	2.416		Crippen Method
mcvol	110.480	ml/mol	McGowan Method
pc	4883.38	kPa	Joback Method
tb	492.62	K	Cheméo Relay (1.0)
tc	730.62	K	Cheméo Relay (1.0)
tf	353.06	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0, beta):

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2493029&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):

Legend

hf:	Enthalpy of formation 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
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point