BORONIC ACID, (4-METHYLPHENYL)-

Other names:	Boronic acid, B-(4-methylphenyl)-
	Boronic acid, p-tolyl-
	p-Tolueneboronic acid
	p-Tolylboronic acid
Inchi:	InChI=1S/C7H9BO2/c1-6-2-4-7(5-3-6)8(9)10/h2-5,9-10H,1H3
InchiKey:	BIWQNIMLAISTBV-UHFFFAOYSA-N
Formula:	C7H9BO2
SMILES:	Cc1ccc(B(O)O)cc1
Mol. weight [g/mol]:	135.96

Physical Properties

Property code	Value	Unit	Source
af	0.7795		Cheméo Relay (1.0)
gf	-241.98	kJ/mol	Cheméo Relay (1.0, beta)
hf	-423.23	kJ/mol	Cheméo Relay (1.0)
hvap	79.54	kJ/mol	Cheméo Relay (1.0)
ie	9.18	eV	Cheméo Relay (1.0)
log10ws	-1.43		Cheméo Relay (1.0)
logp	-0.325		Crippen Method
pc	4919.68	kPa	Cheméo Relay (1.0, beta)
tb	535.94	K	Cheméo Relay (1.0)
tc	771.85	K	Cheméo Relay (1.0)
tf	395.70	K	Cheméo Relay (1.0)
vc	0.396	m3/kmol	Cheméo Relay (1.0)

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5720058&Units=SI
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):	
Solubilities of p-Tolylboronic Acid, Bromobenzene and 4-Phenyltoluene in Carbon Dioxide at Elevated Pressures:	https://www.doi.org/10.1021/je034051y

Legend

af:	Acentric Factor
gf:	Standard Gibbs free energy of formation
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
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume