4-Bromo-2-phenyl phenol

Other names: 5-bromo[1,1'-biphenyl]-2-ol
[1,1'-Biphenyl]-2-ol, 5-bromo-
Inchi: InChI=1S/C12H9BrO/c13-10-6-7-12(14)11(8-10)9-4-2-1-3-5-9/h1-8,14H
InchiKey: AWIYHSVPCXSVRF-UHFFFAOYSA-N
Formula: C12H9BrO
SMILES: Oc1ccc(Br)cc1-c1ccccc1
Mol. weight [g/mol]: 249.10
CAS: 16434-97-2

Physical Properties

Property code	Value	Unit	Source
gf	125.05	kJ/mol	Joback Method
hf	19.60	kJ/mol	Joback Method
hfus	25.60	kJ/mol	Joback Method
hvap	66.97	kJ/mol	Joback Method
log10ws	-4.79		Crippen Method
logp	3.822		Crippen Method
mcvol	155.790	ml/mol	McGowan Method
pc	4414.96	kPa	Joback Method
tb	679.08	K	Joback Method
tc	952.61	K	Joback Method
tf	326.50 ± 0.50	K	NIST Webbook
vc	0.519	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	360.51	J/mol×K	679.08	Joback Method
cpg	412.11	J/mol×K	907.02	Joback Method
cpg	403.09	J/mol×K	861.43	Joback Method
cpg	393.61	J/mol×K	815.84	Joback Method
cpg	383.48	J/mol×K	770.26	Joback Method
cpg	372.50	J/mol×K	724.67	Joback Method
cpg	420.84	J/mol×K	952.61	Joback Method

dvisc	0.0000217	Pa×s	679.08	Joback Method
dvisc	0.0000308	Pa×s	642.88	Joback Method
dvisc	0.0000457	Pa×s	606.68	Joback Method
dvisc	0.0000713	Pa×s	570.48	Joback Method
dvisc	0.0001182	Pa×s	534.28	Joback Method
dvisc	0.0002109	Pa×s	498.08	Joback Method
dvisc	0.0004118	Pa×s	461.88	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	454.00 ± 1.00	K	1.60	NIST Webbook

Sources

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=C16434972&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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
tbrp: Boiling point at reduced pressure

tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume