2-Bromo-4,6-di-tert-butylphenol

Other names:	Phenol, 2-bromo-4,6-bis(1,1-dimethylethyl)-
	2-Bromo-4,6-di-t-butylphenol
Inchi:	InChI=1S/C14H21BrO/c1-13(2,3)9-7-10(14(4,5)6)12(16)11(15)8-9/h7-8,16H,1-6H3
InchiKey:	DIWZVAHZEOFSLS-UHFFFAOYSA-N
Formula:	C14H21BrO
SMILES:	CC(C)(C)c1cc(Br)c(O)c(C(C)(C)C)c1
Mol. weight [g/mol]:	285.22
CAS:	20834-61-1

Physical Properties

Property code	Value	Unit	Source
gf	25.53	kJ/mol	Joback Method
hf	-287.18	kJ/mol	Joback Method
hfus	21.52	kJ/mol	Joback Method
hvap	67.22	kJ/mol	Joback Method
log10ws	-4.81		Crippen Method
logp	4.750		Crippen Method
mcvol	207.730	ml/mol	McGowan Method
pc	2487.55	kPa	Joback Method
tb	696.68	K	Joback Method
tc	938.99	K	Joback Method
tf	475.36	K	Joback Method
vc	0.718	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	551.70	J/mol×K	696.68	Joback Method
cpg	567.42	J/mol×K	737.06	Joback Method
cpg	582.07	J/mol×K	777.45	Joback Method
cpg	595.83	J/mol×K	817.83	Joback Method
cpg	608.86	J/mol×K	858.22	Joback Method
cpg	621.34	J/mol×K	898.60	Joback Method
cpg	633.45	J/mol×K	938.99	Joback Method

dvisc	0.0002806	Pa×s	475.36	Joback Method
dvisc	0.0001348	Pa×s	512.25	Joback Method
dvisc	0.0000715	Pa×s	549.13	Joback Method
dvisc	0.0000411	Pa×s	586.02	Joback Method
dvisc	0.0000252	Pa×s	622.91	Joback Method
dvisc	0.0000163	Pa×s	659.79	Joback Method
dvisc	0.0000111	Pa×s	696.68	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C20834611&Units=SI
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

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