

Phenol, 2-bromo-4-(1,1-dimethylethyl)-

Other names:	2-Bromo-4-tert-butylphenol 4-tert-Butyl-2-Bromophenol
Inchi:	InChI=1S/C10H13BrO/c1-10(2,3)7-4-5-9(12)8(11)6-7/h4-6,12H,1-3H3
InchiKey:	FFRLMQPMGIMHHQ-UHFFFAOYSA-N
Formula:	C10H13BrO
SMILES:	CC(C)(C)c1ccc(O)c(Br)c1
Mol. weight [g/mol]:	229.11
CAS:	2198-66-5

Physical Properties

Property code	Value	Unit	Source
gf	-1.36	kJ/mol	Joback Method
hf	-184.40	kJ/mol	Joback Method
hfus	18.96	kJ/mol	Joback Method
hvap	58.95	kJ/mol	Joback Method
log10ws	-3.50		Crippen Method
logp	3.452		Crippen Method
mvol	151.370	ml/mol	McGowan Method
pc	3786.98	kPa	Joback Method
tb	603.41	K	Joback Method
tc	851.36	K	Joback Method
tf	415.34	K	Joback Method
vc	0.504	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	351.39	J/molxK	603.41	Joback Method
cpg	406.71	J/molxK	810.03	Joback Method
cpg	397.19	J/molxK	768.71	Joback Method
cpg	387.04	J/molxK	727.38	Joback Method
cpg	376.13	J/molxK	686.06	Joback Method
cpg	364.29	J/molxK	644.73	Joback Method
cpg	415.76	J/molxK	851.36	Joback Method

dvisc	0.0000350	Paxs	603.41	Joback Method
dvisc	0.0000516	Paxs	572.06	Joback Method
dvisc	0.0000796	Paxs	540.72	Joback Method
dvisc	0.0001294	Paxs	509.38	Joback Method
dvisc	0.0002243	Paxs	478.03	Joback Method
dvisc	0.0004200	Paxs	446.69	Joback Method
dvisc	0.0008644	Paxs	415.34	Joback Method

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=C2198665&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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

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