

4-Bromo-2-t-butyl phenol

Inchi:	InChI=1S/C10H13BrO/c1-10(2,3)8-6-7(11)4-5-9(8)12/h4-6,12H,1-3H3
InchiKey:	IKMJSWBFODAWTC-UHFFFAOYSA-N
Formula:	C10H13BrO
SMILES:	CC(C)(C)c1cc(Br)ccc1O
Mol. weight [g/mol]:	229.11
CAS:	10323-39-4

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
mcvol	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	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	351.39	J/mol×K	603.41	Joback Method
cpg	364.29	J/mol×K	644.73	Joback Method
cpg	376.13	J/mol×K	686.06	Joback Method
cpg	387.04	J/mol×K	727.38	Joback Method
cpg	397.19	J/mol×K	768.71	Joback Method
cpg	406.71	J/mol×K	810.03	Joback Method
cpg	415.76	J/mol×K	851.36	Joback Method
dvisc	0.0008644	Pa×s	415.34	Joback Method
dvisc	0.0004200	Pa×s	446.69	Joback Method

dvisc	0.0002243	Pa×s	478.03	Joback Method
dvisc	0.0001294	Pa×s	509.38	Joback Method
dvisc	0.0000796	Pa×s	540.72	Joback Method
dvisc	0.0000516	Pa×s	572.06	Joback Method
dvisc	0.0000350	Pa×s	603.41	Joback Method

Sources

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=C10323394&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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