3-Bromophenol, isoBOC

Inchi: InChI=1S/C11H13BrO3/c1-8(2)7-14-11(13)15-10-5-3-4-9(12)6-10/h3-6,8H,7H2,1-2H3
InchiKey: BGVXUCZFFMKOEG-UHFFFAOYSA-N
Formula: C11H13BrO3
SMILES: CC(C)COC(=O)Oc1cccc(Br)c1
Mol. weight [g/mol]: 273.12

Physical Properties

Property code	Value	Unit	Source
gf	-182.52	kJ/mol	Joback Method
hf	-401.28	kJ/mol	Joback Method
hfus	23.64	kJ/mol	Joback Method
hvap	60.63	kJ/mol	Joback Method
log10ws	-4.03		Crippen Method
logp	3.620		Crippen Method
mcvol	172.900	ml/mol	McGowan Method
pc	2915.53	kPa	Joback Method
rinpol	1643.00		NIST Webbook
rinpol	1643.00		NIST Webbook
tb	647.17	K	Joback Method
tc	871.68	K	Joback Method
tf	391.86	K	Joback Method
vc	0.641	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	409.45	J/mol×K	647.17	Joback Method
cpg	466.78	J/mol×K	834.26	Joback Method
cpg	456.95	J/mol×K	796.84	Joback Method
cpg	446.32	J/mol×K	759.42	Joback Method
cpg	434.86	J/mol×K	722.01	Joback Method
cpg	422.58	J/mol×K	684.59	Joback Method
cpg	475.81	J/mol×K	871.68	Joback Method
dvisc	0.0001395	Pa×s	647.17	Joback Method

dvisc	0.0001761	Pa×s	604.62	Joback Method
dvisc	0.0002303	Pa×s	562.07	Joback Method
dvisc	0.0003146	Pa×s	519.52	Joback Method
dvisc	0.0004544	Pa×s	476.96	Joback Method
dvisc	0.0007054	Pa×s	434.41	Joback Method
dvisc	0.0012047	Pa×s	391.86	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R235113&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume